Curve Fitting

Before You Begin

Selecting the Active Data Plot

When performing linear or nonlinear fitting when the graph window is active, you must make the desired data plot the active data plot. To make a data plot active, select the data plot from the data list at the bottom of the **Data** menu. The data list includes all the data plots in the active layer. The currently active data plot is checked.

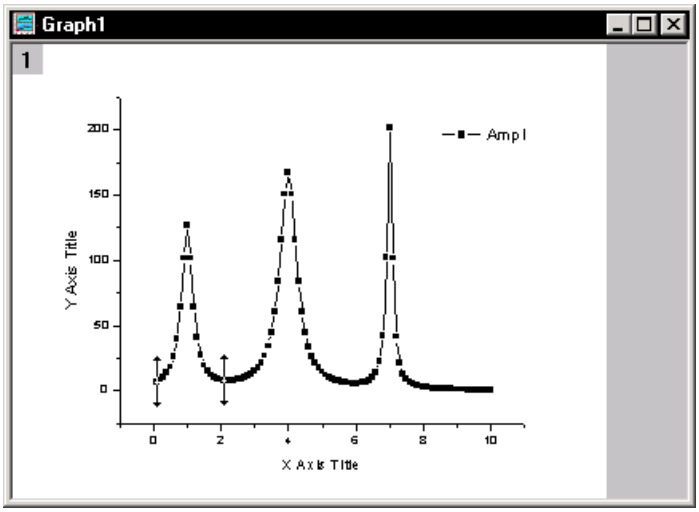
Selecting a Range of a Data Plot

To select a range of a data plot for fitting, click the Data Selector tool on the Tools toolbar. Data markers display at both ends of the active data plot. Additionally, the Data Display tool opens if it is not already open.

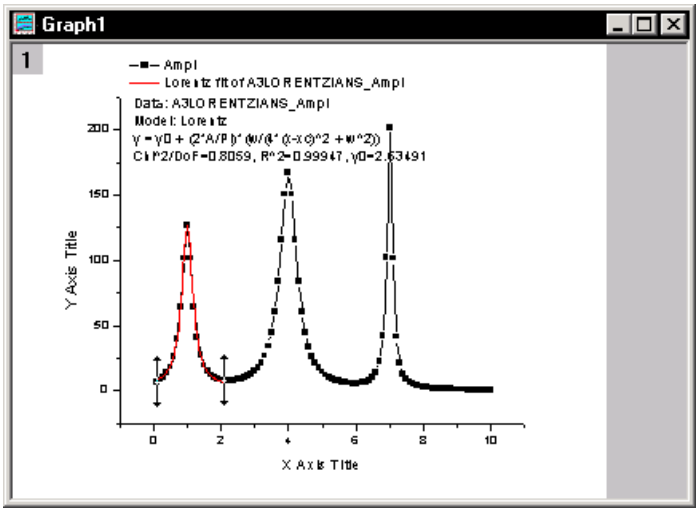
To mark the data segment of interest, click and drag the markers with the mouse. You can also use the left and right arrow keys to select a marker. The CTRL + left or right arrow keys move the selected marker to the next data point. Holding both the SHIFT and CTRL keys while depressing the left or right arrow keys moves the data markers in increments of five along the data plot. (Note: If your X data is not sorted, you may need to sort the data before selecting a range. To do this, activate the worksheet and select **Analysis:Sort Worksheet:Ascending**.)

As with the Data Reader tool, you can press the spacebar to increase the cross hair size.

After you have defined the range of interest, press ESC or click the Pointer button on the Tools toolbar.



Any fitting operations you perform on this data plot will apply to the selected region only.



To hide the data outside this range, select **Data:Set Display Range**.

To remove the selection range, select **Data:Reset to Full Range**.

The Results Log

Origin automatically routes results from most fitting operations to the Results Log. For a complete discussion on the Results Log, see Data Analysis.

Linear Fitting From the Menu

Origin's linear and polynomial fit menu commands are located in the **Analysis** menu. Parameter initialization and linear least squares fitting is carried out automatically when fitting from the menu. A worksheet is created for the fit data, and a fit curve is displayed in the graph window. The fitting parameters and statistical results are recorded in the Results Log.

Linear Regression

To fit a straight line to the active data plot, select **Analysis:Fit Linear**. With the X data, the independent variable, and the Y data, the dependent variable, the estimated linear regression model is stated:

$$Y_i = A + BX_i$$

where the parameters, A and B, are estimated by the method of least squares.

A is the intercept: $A = \overline{Y} - B\overline{X}$

B is the slope: $$B = \frac{\sum_{i}^{N}\left(X_i - \overline{X}\right)\left(Y_i - \overline{Y}\right)}{\sum_{i}^{N}\left(X_i - \overline{X}\right)^2}$$

After the fitting, Origin creates a new (hidden) worksheet containing the fitted data, and plots this data in the active graph window. Additionally, Origin copies the following parameters to the Results Log.

A: Intercept value and its standard error.

B: Slope value and its standard error.

R: Correlation coefficient.

p-value: Probability (that R is zero).

N: Number of data points.

SD: Standard deviation of the fit.

The standard deviation is defined as $\sqrt{\frac{\sum_{i=1}^{N}\left(y_i - (A + Bx_i)\right)^2}{N-2}}$,

where (x_i, y_i) are the data points.

Polynomial Regression

To perform a polynomial fit on the active data plot, select **Analysis:Fit Polynomial**. This menu command opens the Polynomial Fit to *Dataset* dialog box in which you specify the order (1 through 9), number of points drawn in the fit curve, and minimum and maximum X values for the fit curve. To display the fit equation in the graph window, select the Show Formula on Graph check box.

With the X data, the independent variable, and the Y data, the dependent variable, a polynomial regression model of the k^{th} order is stated:

$$Y = A + B_1X + B_2X^2 + B_3X^3 + \ldots + B_kX^k$$

After the fitting, Origin creates a new (hidden) worksheet containing the fitted data, and plots this data in the active graph window. Additionally, Origin copies the following parameters to the Results Log.

A, B_1, B_2, etc.: The parameter estimates and standard errors.

R-square: R-square = (SYY-RSS)/SYY.

p-value: Probability (that R-square is zero).

N: Number of data points.

SD: Standard deviation of the fit.

Multiple Regression

To perform a multiple regression on worksheet data, highlight the independent variable columns and select **Statistics:Multiple Regression**. This menu command opens an Attention dialog box confirming the data set selection and automatic designation. Click OK to perform the multiple regression.

With the first column in the worksheet assumed to contain the dependent variable values (Y), and the highlighted columns assumed to contain the independent variables (X), the multiple regression model is stated:

$$Y = A + B_1 X_1 + B_2 X_2 + \ldots + B_k X_k$$

Origin copies the regression results and the ANOVA table to the Results Log.

A, B_1, B_2, etc.: The parameter estimates and standard errors.

t-value: The t-values for testing if the parameter equals zero, where t = the parameter estimate/standard error of the estimate.

p-value: The corresponding p-values.

R-square: R-square = (SYY-RSS)/SYY.

Adj. R-square: Adj. R-square = 1-[(1-R-square)*(N-1)/(N-k-1)].

Root-MSE: Root-MSE = estimated standard deviation.

Linear Fitting Using the Tools

The Linear Fit Tool

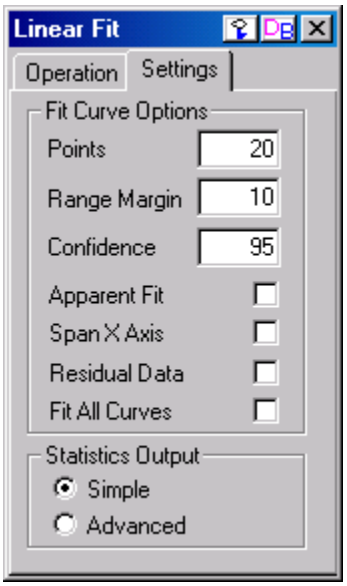
To open the Linear Fit tool, select **Tools:Linear Fit**.

If a worksheet is the active window, you must select a Y column to carry out linear regression. The Y column is used as the dependent variable and the associated X column is used as the independent variable. For weighted fitting, the error bar column must be selected along with the Y column. Note that the data columns must be either of type Numeric or Text & Numeric.

If the graph window is active, the regression is performed on the active data plot. To set the active data plot, select it from the data list at the bottom of the **Data** menu. For weighted fitting, the error bars must be plotted.

Note: To learn more about linear fitting with the Linear Fit tool, review the LINEAR FIT.OPJ project located in your Origin \SAMPLES\ANALYSIS\CURVE FITTING folder.

The Settings Tab



Select this tab to access the Settings options.

The Fit Curve Options Group

Type the number of points to be used in the fit curve data set in the Points text box.

Type the percent outside of the data plot's X value range to create the fit curve (left and right) in the Range Margin text box.

Type the confidence level for calculating confidence and prediction limits in the Confidence text box.

Select the Apparent Fit check box to use the apparent values for fitting, according to the current axis scales. This check box allows you, for example, to fit exponentially decaying data with a straight line fit by plotting the data on a log scale. When this check box is selected and the data has error values associated with it, Origin uses the larger of the positive/negative errors as weight.

Note: To learn more about the apparent fit option, review the APPARENT FIT.OPJ project located in your Origin \SAMPLES\ANALYSIS\CURVE FITTING folder.

Select the Span X Axis check box to calculate a fit curve that spans the entire X axis. The graph is redrawn after fitting to display the entire fit curve over this range.

Select the Residual Data check box to create two columns in the associated data set worksheet. Column Fit(Y) contains the fitting values. Column Residual(Y) contains the residual values.

Select the Fit All Curves check box to fit all the data plots in the layer.

The Statistics Output Group

Select the Simple radio button to output simple fitting statistics to the Results Log, including intercept and slope values and standard errors, R (Correlation Coefficient), Standard Deviation, number of points in the raw data curve, and P (the P value for the t-test of the slope = 0).

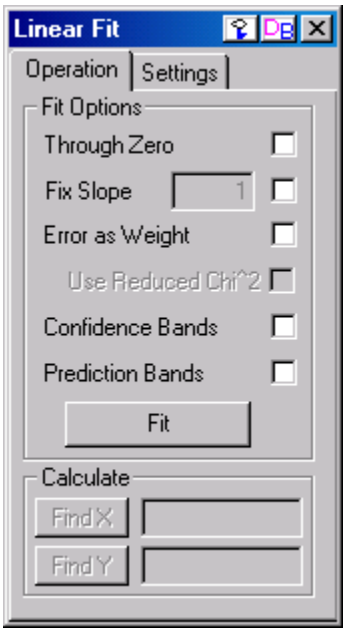
Select the Advanced radio button to output all fitting statistics to the Results Log, including the t-test values and the ANOVA table.

Note: The Linear Fit tool now reports confidence intervals on the fit parameters when the Advanced radio button is selected. The confidence intervals can be checked to determine if their slope is significantly different from unity. If the confidence interval contains the number 1, then the conclusion would be that the slope is not significantly different from unity.

The formula for calculating the confidence intervals on the fit parameters is: (fit parameter value) +/- (standard error on parameter value) * ttable(significance level, degrees of freedom)

The significance level is given by (1- (1-alpha)/2), where alpha is the confidence level. For example, if you set the confidence level in the Linear Fit tool to 95, then the significance level will be (1-(1-0.95)/2) = 0.975. The ttable should then be calculated as ttable(0.975,DOF).

The Operation Tab



Select this tab to access the Operation options.

The Fit Options Group

Select the Through Zero check box to perform a linear regression through the origin when the Fit button is clicked on. When cleared, a standard linear regression is performed.

Select the Fix Slope check box to restrict the slope to the value specified in the Fixed Slope text box on the Settings tab. When cleared, a standard linear regression is performed.Type the fixed slope for the fit curve in the associated text box.

Select the Error as Weight check box to use error bars as weights (1/error^2). If the worksheet is active, a Y error bar column (select **Column:Set as Y Error**) must be selected in addition to the Y column when the Fit button is clicked. If the graph window is active, the error bars must be plotted.

When the Error as Weight check box is selected, the Use Reduced Chi^2 check box becomes available. The Use Reduced Chi^2 check box only affects the error on the parameters reported from the fitting process, and does not affect the fitting process or the data in any way.

When the Use Reduced Chi^2 check box is cleared, the error on the fit parameters is calculated as SQRT(cov_{ii}). This is the default, and recommended setting for this check box.

When the Use Reduced Chi^2 check box is selected, the error on the fit parameters are multiplied by the square root of the reduced chi-squared. In this case, the error on the fit parameters is calculated as SQRT(cov_{ii}*(ChiSqr/DOF)).

Select the Confidence Bands check box to plot upper and lower confidence band data sets with the fitting curve. The confidence band is calculated as $\hat{Y}_{X_0} \pm t(1-\alpha/2, n-2)s\left\{\hat{Y}_{X_0}\right\}$

where $s^2\left\{\hat{Y}_{X_0}\right\} = MSE[1/n + (X_0 - \overline{X})^2 / \sum (X_i - \overline{X})^2]$. $\hat{Y}_{X_0}$ is the unbiased estimator of the expected value of Y at X_0. The band will flare out the further it gets from the mean.

Select the Prediction Bands check box to plot upper and lower prediction band data plots with the fitting curve. The prediction band is calculated as $\hat{Y}_{X_0} \pm t(1-\alpha/2, n-2)s\{pred\}$

where $s^2\{pred\} = MSE + s^2\left\{\hat{Y}_{X_0}\right\}$. $\hat{Y}_{X_0}$ is the unbiased estimator of the expected value of Y at X_0. This band is wider than the confidence band due to $s\{pred\}$.

Click Fit to perform a linear regression on the selected data plot according to the tool settings. If a worksheet is active, the highlighted Y column is used as the dependent variable. The associated X column is used as the independent variable. If a graph window is active, the regression is performed on the active data plot. After the fitting, Origin creates a new (hidden) worksheet containing the fitted data, and plots this data in the active graph window. If the data set has not yet been plotted, a new default graph window opens with the selected Y data set (and its associated X data set, row number, or incremental X value) and fitting data plotted in layer 1. Additionally, Origin displays the fitting results in the Results Log.

When the Simple radio button is selected , the following results are reported:

A: Intercept value and its standard error.

B: Slope value and its standard error.

R: Correlation coefficient.

p-value: Probability (that R is zero).

N: Number of data points.

SD: Standard deviation of the fit.

Additional results are provided when the Advanced radio button is selected. These include the t-values for testing if the parameter equals zero, where t= the parameter estimate/standard error of the estimate, and their corresponding p-values. Additionally, the results include R-square= (SYY-RSS)/SYY, adjusted R-square= 1-[(1-R-square)*(N-1)/(N-2)], and the ANOVA table.

The Calculate Group

The Find X and Find Y buttons allow you to obtain a Y value given an X value, or obtain an X value given a Y value, respectively, from the fit you perform to the data. These buttons become active only after you perform a fit to the active data set.

Once the fit has been performed and the buttons are active, you can enter a numerical value in the top text box next to the Find X button, and then press the Find Y button to obtain the corresponding X value. The exact fit equation that resulted from the fitting process is used to compute the Y value for the given X value. You can specify any X value inside or outside of the range of the data set or the fit line for computing the Y value.

To find an X value for a given Y value, you should enter the Y value in the bottom text box next to the Find Y button and then press Find X. When this action is performed, the X value is determined in the following way:

The fit equation Y = A + B * X is inverted to give X = (Y - A) / B and this inverted equation is used to compute the exact X value for the given Y value. You can specify any Y value inside or outside of the range covered by the data set or the fit line to compute the corresponding X value.

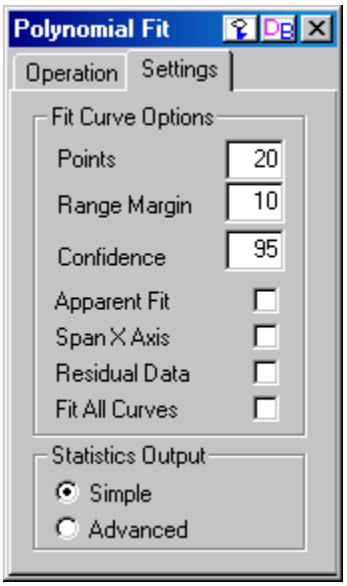
The Polynomial Fit Tool

To open the Polynomial Fit tool, select **Tools:Polynomial Fit**.

If a worksheet is the active window, you must select a Y column to carry out polynomial regression. The Y column is used as the dependent variable and the associated X column is used as the independent variable. For weighted fitting, the Y error bar column must be selected along with the Y column for fitting. Note that the data columns must be either of type Numeric or Text & Numeric.

If the active window is a graph window, the regression is performed on the active data plot. To set the active data plot, select it from the data list at the bottom of the **Data** menu. For weighted fitting, the error bars must be plotted.

The Settings Tab



Select this tab to access the Settings options.

The Fit Curve Options Group

Type the number of points to be used in the fit curve data set in the Points text box.

Type the percent outside of the data plot's X value range to create the fit curve (left and right) in the Range Margin text box.

Type the confidence level for calculating confidence and prediction limits in the Confidence text box.

Select the Span X Axis check box to calculate a fit curve that spans the entire X axis. The graph is redrawn after fitting to display the entire fit curve over this range.

Select the Residual Data check box to create two columns in the associated data set worksheet. Column Fit(Y) contains the fitting values. Column Residual(Y) contains the residual values.

Select the Fit All Curves check box to fit all the data plots in the layer.

The Statistics Output Group

Select the Simple radio button to output simple fitting statistics to the Results Log, including the intercept and B_1, B_2, etc. values and errors, R-Square (Coefficient of Determination), Standard Deviation, number of points in the raw data curve, and P (the P value for R-square = 0).

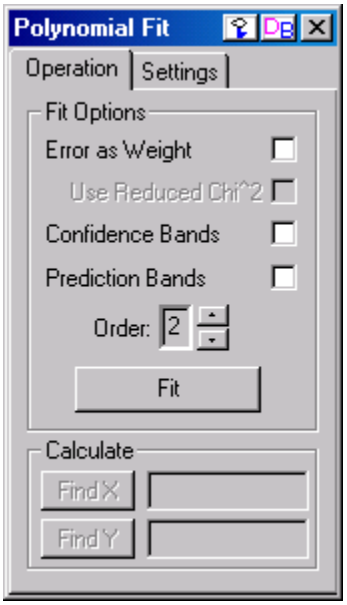
Select the Advanced radio button to output all fitting statistics to the Results Log, including the t values and the ANOVA table.

Note: The Polynomial Fit tool now reports confidence intervals on the fit parameters when the Advanced radio button is selected. The confidence intervals can be checked to determine if their slope is significantly different from unity. If the confidence interval contains the number 1, then the conclusion would be that the slope is not significantly different from unity.

The formula for calculating the confidence intervals on the fit parameters is: (fit parameter value) +/- (standard error on parameter value) * ttable(significance level, degrees of freedom)

The significance level is given by (1- (1-alpha)/2), where alpha is the confidence level. For example, if you set the confidence level to 95, then the significance level will be (1-(1-0.95)/2) = 0.975. The ttable should then be calculated as ttable(0.975,DOF).

The Operation Tab



The Fit Options Group

Select the Error as Weight check box to use error bars as weights (1/error^2). If the worksheet is active, a Y error bar column (select **Column:Set as Y Error**) must be selected in addition to the Y column when the Fit button is clicked. If the graph window is active, the error bars must be plotted.

When the Error as Weight check box is selected, the Use Reduced Chi^2 check box becomes available. The Use Reduced Chi^2 check box only affects the error on the parameters reported from the fitting process, and does not affect the fitting process or the data in any way.

When the Use Reduced Chi^2 check box is cleared, the error on the fit parameters is calculated as SQRT(cov_{ii}). This is the default, and recommended setting for this check box.

When the Use Reduced Chi^2 check box is selected, the error on the fit parameters are multiplied by the square root of the reduced chi-squared. In this case, the error on the fit parameters is calculated as SQRT(cov_{ii}*(ChiSqr/DOF)).

For the polynomial fit, the confidence band is calculated as $\hat{Y}_{X_0} \pm t(1-\alpha/2, n-k)s\left\{\hat{Y}_{X_0}\right\}$ where $s^2\left\{\hat{Y}_{X_0}\right\} = MSE[1/n + (X_0 - \overline{X})^2 / \sum (X_i - \overline{X})^2]$. $\hat{Y}_{X_0}$ is the unbiased estimator of the expected value of Y at X_0. The prediction band is calculated as $\hat{Y}_{X_0} \pm t(1-\alpha/2, n-k)s\{pred\}$ where $s^2\{pred\} = MSE + s^2\left\{\hat{Y}_{X_0}\right\}$. $\hat{Y}_{X_0}$ is the unbiased estimator of the expected value of Y at X_0.

Set the order for the regression, ranging from one to nine, using the Order spin buttons.

Click Fit to perform a polynomial regression on the selected data plot according to the tool settings. If a worksheet is active, the highlighted Y column is used as the dependent variable. The associated X column is used as the independent variable. If a graph window is active, the regression is performed on the active data plot. After the fitting, Origin creates a new (hidden) worksheet containing the fitted data, and plots this data in the active graph window. If the data set has not yet been plotted, a new default graph window opens with the selected Y data set (and its associated X data set, row number, or incremental X value) and fitting data plotted in layer 1. Additionally, Origin displays the fitting results in the Results Log.

When the Simple radio button is selected, the fitting results are:

A, B_1, B_2, etc.: The parameter estimates and standard errors.

R-square: R-square = (SYY-RSS)/SYY.

p-value: Probability (that R-square is zero).

N: Number of data points.

SD: Standard deviation of the fit.

Additional results are provided when the Advanced radio button is selected. These include the t-values for testing if the parameter equals zero, where t= the parameter estimate/standard error of the estimate, and their corresponding p-values. Additionally, the results include R-square= (SYY-RSS)/SYY, adjusted R-square= 1-[(1-R-square)*(N-1)/(N-k-1)], and the ANOVA table.

The Calculate Group

The Find X and Find Y buttons allow you to obtain a Y value given an X value, or obtain an X value given a Y value, respectively, from the fit you perform to the data. These buttons become active only after you perform a fit to the active data set.

Once the fit has been performed and the buttons are active, you can enter a numerical value in the top text box next to the Find X button, and then press the Find Y button to obtain the corresponding X value. The

exact fit equation that resulted from the fitting process is used to compute the Y value for the given X value. You can specify any X value inside or outside of the range of the data set or the fit line for computing the Y value.

To find an X value for a given Y value, you should enter the Y value in the bottom text box next to the Find Y button and then press Find X. When this action is performed, an iterative procedure is used to find the X value corresponding to the given Y value:

1) First a check is performed to see if the Y value you specified is inside the range of Y values corevered by the fit line. If not, no computation is done and you are informed that your Y value is out of range.

2) If the Y value passes this check, then the following steps are performed:

=> The fit line data set is scanned to find two points (X1,Y1) and (X2, Y2) such that the user-specified Y value lies in the interval [Y1, Y2]. In the case of a fit line that is not monotonic (.ie. multiple X value exist for same Y value), the first interval that satisfies this criterion, starting from the lower end of the X axis, is selected.

=> The X value of the mid point of this interval is computed: Xm = (X1 + X2) / 2, and the corresponding y-value, Ym, is computed using the exact fit equation

=> The interval to the right or left of this midpoint is chosen such that the user-specified Y value now falls within the new interval.

=> This bisectional search is continued till the y-value of the mid point of the interval, Ym, differs from the user-specified Y-value by less than 0.00001%, or until 200 iterations are performed, whichever comes first.

=> The Xm value corresponding to the final Ym value is reported as the X value corresponding to the y-value you specified.

A Note on Linear Fitting Theory

Theory of Linear Regression

For a given dataset (x_i , y_i), i = 1,2,...N, we assign X as the independent variable and Y as the dependent variable. Assume the residuals $res_i = y_i - (a + bx_i)$ have normal (Gaussian) distributions with the mean = 0 and the variance = σ_i^2 . The maximum likelihood estimates for the parameters a and b can be obtained by minimizing the chi-square $\chi^2 = \sum_{i=1}^{N} \frac{[y_i - (a + bx_i)]^2}{\sigma_i^2} = \sum_{i=1}^{N} w_i \left[y_i - (a + bx_i)\right]^2$. This is essentially a weighted sum of squares with weights $w_i = \frac{1}{\sigma_i^2}$. Using the Linear Regression toolbar, you can set $w_i = \frac{1}{s_i^2}$, where s_i is the error bar for y_i . If you do not make this choice, Origin will carry out a fitting with equal weights, assuming all the σ_i are equal. This can be done by setting $\sigma_i = 1$.

Define the following variables:

$$sxy = \sum_{i=1}^{n} w_i x_i y_i \ , \ sxx = \sum_{i=1}^{n} w_i x_i^2 \ , \ syy = \sum_{i=1}^{n} w_i y_i^2 \ , \ sx = \sum_{i=1}^{n} w_i x_i \ , \ sy = \sum_{i=1}^{n} w_i y_i$$

$$SXY = \sum_{i=1}^{n} w_i (x_i - \bar{x})(y_i - \bar{y}) \ , \ SXX = \sum_{i=1}^{n} w_i (x_i - \bar{x})^2 \ , \ SYY = \sum_{i=1}^{n} w_i (y_i - \bar{y})^2$$

where the mean for X and Y are given by $\bar{x} \equiv \frac{sx}{wTotal}$, $\bar{y} \equiv \frac{sy}{wTotal}$, and $wTotal = \sum_{i=1}^{n} w_i$.

The correlation coefficient is $r = \frac{SXY}{\sqrt{SXX}\sqrt{SYY}}$.

Fitting to a Straight Line with Intercept: Y=a+bX

1. The estimated parameters are $\mathrm{b} = \frac{SXY}{SXX}$, and $a = \bar{y} - b\bar{x}$ with standard errors $se(b) = \frac{sd}{\sqrt{SXX}}$, and $se(a) = sd\sqrt{\left(\frac{1}{wTotal} + \frac{\bar{x}^2}{SXX}\right)}$. $sd = \sqrt{\frac{RSS}{df}}$ is the estimated standard deviation of the fitting and df = n - 2. The residual sum of squares is $RSS = \sum_{i=1}^{n} w_i [y_i - (a + bx_i)]^2$.

2. The $(1-\alpha)\times 100\%$ confidence interval (confidence band) for the mean of Y is given by: $Y = bx \pm t(\alpha/2, n-2)\, sd\sqrt{\frac{1}{wTotal} + \frac{(x-\bar{x})^2}{SXX}}$.

3. The coefficient of determination is $COD = 1 - \frac{RSS}{SYY}$. COD is also called R-squared since COD = r^2. The adjusted R-squared is $R^2_{adj} = 1 - [1 - r^2]\frac{n-1}{df}$.

4. The ANOVA for the fitting is summarized in the following table:

	Degree of Freedom	Sum of Squares (SS)	Mean Squares (MS)	F
Regression	1	SSreg=SYY-RSS	MSreg=SSreg/1	MSreg/MSE
Residual	n-2	RSS	MSE=RSS/(n-2)	
Total	n-1	SYY		

The variable F=MSreg/MSE follows an F distribution F(1,n-2). The P-value can be obtained from the F distribution.

Fitting to a Straight Line Through the Origin: Y=bX

1) The estimated parameter is $\mathrm{b} = \frac{sxy}{sxx}$, with standard error $se(b) = \frac{sd}{\sqrt{sxx}}$. $sd = \sqrt{\frac{RSS}{df}}$ is the estimated standard deviation of the fitting, df = n - 1, and the residual sum of squares is $RSS = \sum_{i=1}^{n} w_i [y_i - bx_i]^2$.

2) The $(1-\alpha)\times 100\%$ confidence interval (confidence band) for the mean of Y is given by: $Y = a + bx \pm t(\alpha/2, n-1)\, sd \sqrt{\frac{x^2}{sxx}}$.

3) The ANOVA for the fitting is summarized in the following table:

	Degree of Freedom	Sum of Squares (SS)	Mean Squares (MS)	F
Regression	1	SSreg=SYY-RSS	MSreg=SSreg/1	MSreg/MSE
Residual	n-1	RSS	MSE=RSS/(n-1)	
Total	n	SYY		

The variable F=MSreg/MSE will follow an F distribution F(1,n-1). The P-value can be obtained from the F distribution.

Theory of Polynomial Regression

To fit a polynomial of order k ($Y = b_0 + b_1 X + b_2 X^2 + \ldots\ldots + b_k X^k$) to the data, assume the residuals $res_i = y_i - (b_0 + b_1 x_i + b_2 x_i^2 + \ldots\ldots + b_k x_i^k)$ have normal (Gaussian) distributions with the mean = 0 and the variance = σ_i^2. Then the maximum likelihood estimates for the parameters b[i] can be obtained by minimizing the chi-square $\chi^2 = \sum_{i=1}^{N} \frac{res_i^2}{\sigma_i^2} = \sum_{i=1}^{N} w_i res_i^2$. Origin uses equal weight fitting by setting $\sigma_i = 1$.

1) The estimated parameters can be expressed in matrix form: $b = (\tilde{A}A)^{-1}\tilde{A}Y$, where

$$b = \begin{bmatrix} b_0 \\ b_1 \\ \\ \\ b_k \end{bmatrix},\ A = \begin{bmatrix} \frac{1}{\sigma_1} & & \frac{x_1^k}{\sigma_1} \\ & & \\ & & \\ \frac{1}{\sigma_n} & & \frac{x_n^k}{\sigma_n} \end{bmatrix},\ Y = \begin{pmatrix} \frac{y_1}{\sigma_1} \\ \\ \\ \frac{y_n}{\sigma_n} \end{pmatrix}$$

The residual sum of squares is $RSS = \sum_{i=1}^{N} w_i res_i^2$. The estimated standard deviation of the fitting is $sd = \sqrt{\frac{RSS}{df}}$, and df = n - (k + 1).

2) The ANOVA for the fitting is summarized in the following table:

	Degree of Freedom	Sum of Squares (SS)	Mean Squares (MS)	F
Regression	k	SSreg=SYY-RSS	MSreg=SSreg/k	MSreg/MSE
Residual	n-(k+1)	RSS	MSE=RSS/(n-k-1)	
Total	n-1	SYY		

The variable F=MSreg/MSE will follow an F distribution F(k,df). The P-value can be obtained from the F distribution.

Theory of Multiple Regression

For given columns of data $\left(Y[i] \quad X_1[i] \quad X_2[i] \qquad X_k[i]\right)$, i = 1,2,...N, we assign the Y column to be the dependent variable, and all other X columns to be the independent variables. We fit the model: $Y = b_0 + b_1 X_1 + \ldots\ldots + b_k X_k$, assuming the residuals $res_i = y_i - (b_0 + b_1 x_{1i} + b_2 x_{2i} + \ldots\ldots + b_k x_{ki})$ have normal (Gaussian) distributions with the mean = 0 and the variance = σ^2. Then the maximum likelihood estimation for the parameters b[i] can be obtained by minimizing the chi-square $\chi^2 = \sum_{i=1}^{N} res_i^2$.

1) The estimated parameters can be expressed in matrix form: $b = (\tilde{A}A)^{-1}\tilde{A}Y$

$$b = \begin{bmatrix} b_0 \\ b_1 \\ \\ \\ b_k \end{bmatrix},\ A = \begin{bmatrix} 1 & x_{11} & & x_{k1} \\ & & & \\ & & & \\ & & & \\ 1 & x_{n1} & & x_{kn} \end{bmatrix},\ Y = \begin{pmatrix} y_1 \\ \\ \\ \\ y_n \end{pmatrix}$$

The residual sum of squares is $RSS = \sum_{i=1}^{N} res_i^2$.

2) $sd = \sqrt{\frac{RSS}{df}}$ is the estimated standard deviation of the fitting and df = n - (k + 1).

3) The ANOVA for the fitting is summarized in the following table:

	Degree of Freedom	Sum of Squares (SS)	Mean Squares (MS)	F
Regression	k	SSreg=SYY-RSS	MSreg=SSreg/k	MSreg/MSE
Residual	n-(k+1)	RSS	MSE=RSS/(n-k-1)	
Total	n-1	SYY		

The variable F=MSreg/MSE will follow an F distribution F(k,df). The P-value can be obtained from the F distribution.

Nonlinear Curve Fitting from the Menu

The **Analysis** menu includes commands which use nonlinear least squares fitting to generate a fit curve in the graph window. The fitting parameters, as well as related statistics, are displayed in the Results Log.

First Order Exponential Decay

Select **Analysis:Fit Exponential Decay:First Order** to fit a curve to the active data plot, using the equation:

$y = y_0 + A_1 e^{-x/t_1}$, where

y_0 Y offset

A_1 amplitude

t_1 decay constant

When you select this menu command, Origin makes the necessary initialization for the parameters. Origin also sets y_0 to an appropriate fixed number which is close to the asymptotic value of the Y variable for large X values.

Note: When fitting from the menu, all the parameters by default vary during the iterative procedure. If you want to fix certain parameters to particular values, you must open the curve fitter's dialog box.

Second Order Exponential Decay

Select **Analysis:Fit Exponential Decay:Second Order** to fit a curve to the active data plot, using the equation:

$$y = y_0 + A_1 e^{-x/t_1} + A_2 e^{-x/t_2}$$

This menu command opens the Verify Initial Guesses dialog box in which you specify initial values for the fitting parameters.

Fitting to multiple exponentials is more difficult than fitting to a single exponential. You must make good guesses for the fitting parameters. You may need to enter the nonlinear fitting session to get better control for the fitting.

Note: To learn more about second order exponential decay fitting, review the EXP DECAY.OPJ project located in your Origin \SAMPLES\ANALYSIS\CURVE FITTING folder.

Third Order Exponential Decay

Select **Analysis:Fit Exponential Decay:Third Order** to fit a curve to the active data plot, using the equation:

$$y = y_0 + A_1 e^{-x/t_1} + A_2 e^{-x/t_2} + A_3 e^{-x/t_3}$$

This menu command opens the Verify Initial Guesses dialog box in which you specify initial values for the fitting parameters.

Exponential Growth

Select **Analysis:Fit Exponential Growth** to fit a curve to the active data plot, using the equation:

$y = y_0 + A_1 e^{x/t_1}$, where

y_0 Y offset

A_1 amplitude

t_1 "time" constant

Gaussian

Select **Analysis:Fit Gaussian** to fit a curve to the active data plot, using the equation:

$$y = y_0 + \frac{A}{w \cdot \sqrt{\frac{\pi}{2}}} e^{-\frac{2(x-x_0)^2}{w^2}}$$

, where

y_0 baseline offset

A total area under the curve from the baseline

x_0 center of the peak

w 2 "sigma", approximately 0.849 the width of the peak at half height

This model describes a bell-shaped curve like the normal (Gaussian) probability distribution function. The center x_0 represents the "mean", while $w/2$ is the standard deviation.

Lorentzian

Select **Analysis:Fit Lorentzian** to fit a curve to the active data plot, using the equation:

$$y = y_0 + \frac{2 \cdot A}{\pi} \cdot \frac{w}{4(x - x_0)^2 + w^2}$$

, where

y_0 baseline offset

A total area under the curve from the baseline

x_0 center of the peak

w full width of the peak at half height

The parameters in the Lorentzian model are similar to the parameters defined for the Gaussian model.

Sigmoidal

Select **Analysis:Fit Sigmoidal** to fit a curve to the active data plot using either the Boltzmann or Logistical equation.

Boltzmann Equation

When the X axis is set to linear scale, the **Analysis:Fit Sigmoidal** menu command uses the Boltzmann equation for fitting:

$$y = \frac{A_1 - A_2}{1 + e^{(x - x_0)/dx}} + A_2$$, where

x_0 center

dx width

A_1 initial Y value: $y(-\infty)$

A_2 final Y value: $y(+\infty)$

The Y value at x_0 is half way between the two limiting values A_1 and A_2: $y(x_0) = (A_1 + A_2)/2$. The Y value changes drastically within a range of the X variable. The width of this range is approximately *dx*.

Logistical Equation

When the X axis is set to a logarithmic scale, the **Analysis:Fit Sigmoidal** menu command uses the Logistical equation for fitting:

$$\frac{A_1 - A_2}{1 + (x / x_0)^p} + A_2$$, where

x_0 center

p power

A_1 initial Y value

A_2 final Y value

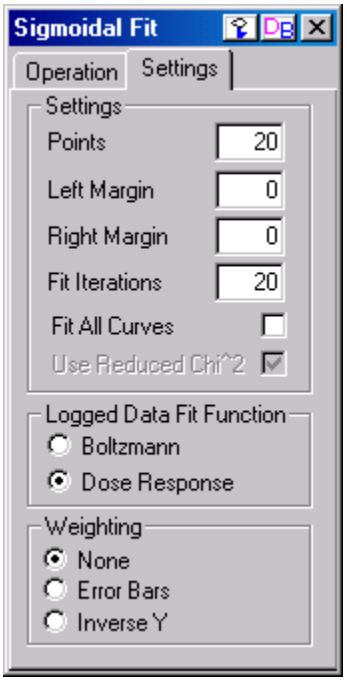
The Y value at x_0 is half way between the two limiting values A_1 and A_2: $y(x_0) = (A_1 + A_2)/2$.

Using the Sigmoidal Fit Tool

To open the Sigmoidal Fit tool, select **Tools:Sigmoidal Fit**. The Sigmoidal Fit tool provides an intermediate level of sophistication for Sigmoidal fitting that is more advanced than the **Analysis:Fit Sigmoidal** menu command and simpler than the **Analysis:Non-Linear Curve Fit:Advanced Fitting Tool** menu command. The fitting function used depends on the X axis scale type and the selected radio button in the Logged Data Fit Function group on the Settings tab.

Note: To learn more about fitting with the Sigmoidal Fit tool, review the SIGMOIDAL FIT.OPJ project located in your Origin \SAMPLES\ANALYSIS\CURVE FITTING folder.

The Settings Tab



Select this tab to access the Settings options.

The Fit Curve Options Group

Specify the number of points to create for the fit curve, the percent outside of the X value range to create the fit curve (left and right), and the number of iterations of the fitting to perform in the associated text boxes. You can also select the Fit All Curves check box to fit all the data plots in a layer.

The Use Reduced Chi^2 check box only affects the error on the parameters reported from the fitting process, and does not affect the fitting process or the data in any way.

Leave the Reduced Chi^2 check box selected when there are no associated error bars with the data (which is the default - and only - option). In this case, the error on the fit parameters is calculated as SQRT(cov_{ii}*(ChiSqr/DOF)).

Leave the check box cleared when the data has associated error bars and a weighting method other than None has been chosen by you. This is the default, and recommended setting for this check box. The error on the fit parameter is then calculated as SQRT(cov_{ii}).

When the data has associated error bars and a weighting method has been chosen by you, you have the option to select the check box, thereby multiplying the reported error on the fit parameters by the square root of the reduced chi-squared. In this case, the error on the fit parameters is calculated as SQRT(cov_{ii}(ChiSqr/DOF)).

The Logged Data Fit Function Group

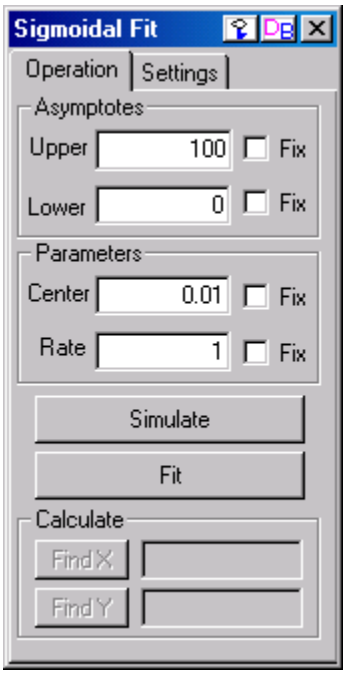
Select either the Boltzmann or Dose Response (logistic) function to fit logged data (for example, 10^7 plotted as 7).

Note: If the X axis scale is set to Log10, the Dose Response (logistic) function is always used, independent of your radio button selection.

The Weighting Group

Select the None, Error Bars, or Inverse Y weighting radio button. If you select the Error Bars radio button, you must have selected a Y error bar column with your Y column in a worksheet, or plotted your data with error bars in a graph. In this case, Origin uses 1/errbar^2 as the weighting. For inverse Y weighting, Origin uses 1/Y where Y is the data that is being fitted to.

The Operation Tab



Select this tab to access the Operations options.

The Asymptotes Group and Associated Fix Check Boxes

Specify the parameters *A1* and *A2* in the Upper and Lower text boxes to be used as the initial values for fitting. Select the associated Fix check boxes to lock in the entered value as a constant rather than allowing it to vary during fitting.

The Parameters Group and Associated Fix Check Boxes

Specify the initial value for the parameter *x0* in the Center text box. Specify the initial value for the parameter *dx* or *p* in the Rate text box. Select the associated Fix check boxes to lock in the entered value as a constant.

The Fit Button

Click Fit to execute the fitting routine and update the variables that have not been set to fixed.

The Simulate Button

If you have specified the values for the parameters and a graph window is active, click Simulate to create a function that can be used like any other function. This can also help you to better determine the initial parameter values for the fit. You can double-click on the function curve or select the function in the data list at the bottom of the **Data** menu (select the function from the data list twice, as the first action simply makes the function the active data set). Both actions open the Function tab of the Plot Details dialog box.

The Calculate Group

The Find X and Find Y buttons allow you to obtain a Y value given an X value, or obtain an X value given a Y value, respectively, from the fit you perform to the data. These buttons become active only after you perform a fit to the active data set.

Once the fit has been performed and the buttons are active, you can enter a numerical value in the top text box next to the Find X button, and then press the Find Y button to obtain the corresponding X value. The exact fit equation that resulted from the fitting process is used to compute the Y value for the given X value. You can specify any X value inside or outside of the range of the data set or the fit line for computing the Y value.

To find an X value for a given Y value, you should enter the Y value in the bottom text box next to the Find Y button and then press Find X. When this action is performed, an iterative procedure is used to find the X value corresponding to the given Y value:

1) First a check is performed to see if the Y value you specified is inside the range of Y values corevered by the fit line. If not, no computation is done and you are informed that your Y value is out of range.

2) If the Y value passes this check, then the following steps are performed:

=> The fit line data set is scanned to find two points (X1,Y1) and (X2, Y2) such that the user-specified Y value lies in the interval [Y1, Y2]. In the case of a fit line that is not monotonic (.ie. multiple X value exist for same Y value), the first interval that satisfies this criterion, starting from the lower end of the X axis, is selected.

=> The X value of the mid point of this interval is computed: Xm = (X1 + X2) / 2, and the corresponding y-value, Ym, is computed using the exact fit equation

=> The interval to the right or left of this midpoint is chosen such that the user-specified Y value now falls within the new interval.

=> This bisectional search is continued till the y-value of the mid point of the interval, Ym, differs from the user-specified Y-value by less than 0.00001%, or until 200 iterations are performed, whichever comes first.

=> The Xm value corresponding to the final Ym value is reported as the X value corresponding to the y-value you specified.

Fitting a Data Plot with Multiple Peaks

Origin includes a number of options for peak analysis including the Baseline tool, the Pick Peaks tool, and the **Analysis:Fit Multi-peaks** menu command. For more information on the Baseline and Pick Peaks tools, see Data Analysis.

Note: To learn more about fitting data with multiple peaks, review the MULTI PEAK FIT.OPJ project located in your Origin \SAMPLES\ANALYSIS\CURVE FITTING folder.

Multiple Gaussian

Select **Analysis:Fit Multi-peaks:Gaussian** to fit a curve with multiple Gaussian peaks to the active data plot. This menu command opens the Number of Peaks dialog box in which you type a value for the

number of peaks. Click OK to close the dialog box. This action opens the Initial Half Width Estimate dialog box. Additionally, Origin estimates the overall half-width through integration, and then divides by the number of peaks to arrive at the half-width estimate. Modify or accept the estimated value in the Initial Half Width Estimate dialog box. Click OK to close the dialog box. The Data Display tool opens if not already open. To read the XY coordinates of a data point in the Data Display tool, click on the desired point. To determine a peak position, double-click (or click + ENTER) on a data point. When complete, the fitting parameters, as well as related statistics, are displayed in the graph window and the Results Log. Additionally, the fit data is copied to a new (hidden) worksheet.

Multiple Lorentzian

Select **Analysis:Fit Multi-peaks:Lorentzian** to fit a curve with multiple Lorentzian peaks to the active data plot. This menu command is similar to the **Multiple Gaussian** menu command as it allows you to specify the number of peaks, and then invokes fitting to multiple Lorentzian functions.

The Fit Comparison Tool

A Fit Comparison tool is available by selecting **Tools:Fit Comparison**. This tool compares two data sets by fitting the same function to the data. It then uses an F-test to determine whether the two data sets are significantly different from each other. Thus, the tool determines if the two data sets are representative samples from the same population or not. The results are output to the Results Log.

The Fit Comparison tool uses the following procedure to perform the comparison:

1) Origin fits the two data sets individually using the selected function. Origin then combines the two data sets (appending one to the other), and then performs a fit on the combined data set with the same function. From these three fits, Origin obtains values for the SSR (sum of squares of the difference between the data and fit values) and the DOF (number of degrees of freedom). Thus, the following values are obtained: SSR1, DOF1, SSR2, DOF2 from the individual fits, and SSRcombined and DOFcombined from the fit to the combined data.

2) Origin then computes the following:

SSRseparate = SSR1 + SSR2

DOFseparate = DOF1 + DOF2

3) Origin then computes an F value using the formula:

$$F = \frac{(SSRcombined - SSRseparate)/(DOFcombined - DOFseparate)}{SSRseparate/DOFseparate}$$

4) Once the F value is computed, Origin calculates a p-value using the formula:

$$p = 1 - invf(F, (DOFcombined - DOFseparate), DOFseparate)$$

This p-value is then used to make a statistical statement as to whether the data (not the parameter values) are significantly different or not. If the p-value is greater than 0.05, we can say that the data sets are not significantly different at the 95% confidence level.

The NLSF Wizard

Origin provides a wizard for performing nonlinear least squares fitting. The NLSF wizard is easier to use than the advanced fitting tool (NLSF), as it steps you through the fitting process. The wizard provides only the most frequently used fitting options. For complete fitting options, open the NLSF. For more information on the NLSF, see "The Nonlinear Least Squares Fitter" on page 536.

Note: If you want to k data from fitting, you must mask the data before opening the NLSF wizard.

To open the NLSF Wizard, select **Analysis:Nonlinear Curve Fit:Fitting Wizard**.

To navigate through the NLSF Wizard, click the Next (and Back) buttons, or click the page icons on the wizard map located on the left side of the wizard. The page icons on the wizard map are color-coded to indicate the active page (green), a page that has not been visited (yellow), a page that has already been visited or skipped (brown), and the last wizard page (red).

The NLSF Wizard includes the following pages:

Select Data: This page contains controls for selecting the Y fitting data set and for selecting a range of data for fitting. You can also select the data plot type and the X axis scale type on this page and on later pages.

Select Function: This page provides controls to select your fitting function. You can browse through functions in the selected category using the Previous and Next buttons located in the Preview window, or you can scroll the Function list to select a function. Additionally, you can add new categories and add / remove functions from categories. You can also delete and rename categories.

Peaks: This page is only available if you have selected a peak function and you select the Multiple Peaks check box. Use this page to initialize peak heights and centers for data sets with multiple peaks. This process is similar to the **Analysis:Fit Multipeaks** menu command. (For data sets with a single peak, Origin will automatically tialize the parameter values.)

Weighting: This page allows you to specify how different data points are to be weighted when computing the reduced chi-square value during the iterative process. To learn about the weighting methods, see "Before you Start: The Chi-Square Minimization" on page 547.

Fitting Control: This page allows you to control the fitting procedure and perform the fit. You can specify the desired confidence level for the confidence and prediction bands, the maximum number of iterations to perform, and the tolerance for performing additional iterations. You can calculate the reduced chi-square value for the current parameter values and perform iterations on this page. After performing the iterations, the reduced chi-square value and the actual number of iterations performed are listed in the Iteration Results view box. For more information on these options, see "Controlling the Fitting Procedure" on page 577.

Results: This page provides controls for outputting the fit curve, residuals, confidence and prediction bands, and fit results label to the active graph or to a new graph. It also provides controls for outputting the parameter results. For more information, see "The Fitting Results" on page 573.

The Results page also provides a Save Fitting Session as a Procedure File check box. For more information on this check box, see "Creating a Custom Wizard" on page 534.

The following buttons are available on the NLSF Wizard:

Enlarge a section of the wizard graph.

Return the wizard graph to the previous enlarged view or back to the full axes scale if the graph was enlarged once.

Scroll the wizard graph axes left, right, up, and down after enlarging.

Return the wizard graph to the full axes scale.

Opens a dialog box for manually initializing the parameter values, fixing parameter values, sharing parameters, and setting parameter constraints including upper and lower bounds and general linear constraints. This dialog box also provides controls for calculating the reduced chi-square value for the current parameter values and for performing Levenberg-Marquardt and Simplex iterations.

Display the residual plot.

Display confidence bands.

Display prediction bands.

Note: A number of wizard settings are saved globally. These include the tolerance and iterations settings which are saved to the NLSF.INI file. Additionally, the confidence and prediction settings, as well as many other wizard settings, are saved as global settings in the NLSFWizard.INI file. Open either initialization file in a text editor to view the settings.

Creating a Custom Wizard

After you become familiar with the NLSF wizard, you might find that you consistently perform the same actions on some wizard pages and no actions on other wizard pages. If you step through the wizard pages in a similar way when fitting data, you can simplify the wizard by hiding pages that you either perform no actions on or ones that you always perform the same actions on. You can then save this customized wizard to a new toolbar button for future access.

To hide a page in the wizard, right-click on a blank section of the wizard (for example, beneath the wizard map) and select **View Mode:Full**. The Full view mode is a wizard design mode. This view mode allows you to turn off the display of wizard pages by clearing the associated check box located on the wizard map.

Now you can step through the wizard specifying which pages you want to hide.

=> To hide a page that you never perform any actions on, clear the associated check box on the wizard map.

=> To hide a page that you want to perform the same actions on, manually perform the action on the page (for example, click the Iterate button on the Fitting Control page) and then clear the page's check box on

the wizard map. When this page is skipped when you run your customized wizard, the wizard will automatically perform the action.

The following actions can be saved to a custom wizard:

Select Data page: No actions are saved on this page. However, you can hide and skip this page because the active data set is used by default.

Select Function page: No actions are saved on this page. Thus, you cannot hide and skip this page.

Peaks page: No actions are saved on this page. You can only hide and skip this page if your data set has a single peak.

Weighting page: This page can only be hidden and skipped if your weighting method is set to None, Instrumental, or Statistical - because Arbitrary and Direct require a data set selection.

Fitting Control page: This page can be hidden and skipped. However, only the Iteration button is recorded. The Chi^2 button is non-recordable.

The following settings are saved to the NLSF.INI file:
Tolerance
Default for the Iterations drop- down list and button

The following settings are saved to the NLSFwizard.INI file:
Confidence Spin/Edit
Prediction Spin/Edit

Results page: You cannot hide and skip this page.

Note: A number of settings are saved globally and are independent of custom wizards. These include the tolerance and iterations settings which are saved to the NLSF.INI file. Additionally, the confidence and prediction settings, as well as many other wizard settings, are saved as global settings in the NLSFWizard.INI file. Open either initialization file in a text editor to view the settings.

After clearing the desired wizard map check boxes, perform the following steps to create your custom wizard:

1) On the Results page, select the Save Fitting Session as a Procedure File check box.

2) Right-click again on a blank section of the wizard and select **View Mode:Normal** from the shortcut menu. The wizard map updates displaying only the non-hidden pages.

3) Click the Finish button. This action opens the Button Settings dialog box.

This dialog box allows you to save your current wizard settings and actions to a new toolbar button.

When the Button Settings dialog box opens after you click the wizard's Finish button, the top left button in the dialog box will be depressed. You can assign your custom wizard settings to this button or you can select another button. Note: This dialog box does not recognize if a bitmap button is already in use.

You can specify a ToolTip and status bar message for your button.

After you click the OK button, Origin adds this button to a new NLSFWiz toolbar.

The Nonlinear Least Squares Fitter

One of the most powerful and complex components of Origin is its nonlinear least squares fitting (NLSF) capability. Using the nonlinear least squares fitter you can fit a function, or a set of functions, to your data, depending on one (or several) independent variables and up to 200 fitting parameters. Essentially, the only limitation is the memory of your computer. Origin provides nearly 200 built-in functions selected from different areas of research and development. Should you be unable to find the function you require among the built-in functions, define a function and Origin will fit it to your data.

Origin's nonlinear regression method is based on the Levenberg-Marquardt (LM) algorithm and is the most widely used algorithm in nonlinear least squares fitting. The Simplex minimization method is provided as well.

Origin’s nonlinear least squares curve fitter is very flexible. It enables you to take almost full control of the fitting process:

1) Estimate initial parameter values by one of three methods: (i) plotting the curve before the actual fitting and comparing it to the data, (ii) use Origin’s automatic parameter initialization feature (built-in functions

only) or (iii) write your own Origin C code to calculate dataset-specific parameter estimates for your user-defined functions

2) Impose linear constraints on the values of parameters.

3) Monitor the relevant quantities during the iterative process which may indicate ill-behaving functions.

4) Select the weighting method.

5) Easily set the fitting data range, etc.

Note: The NLSF always reports the reduced chi^2 value, not chi^2. In some locations of the NLSF, reduced chi^2 is labeled "chi^2". In other locations, it is labeled "chi^2/DoF". In all cases the actual value is reduced chi^2.

Entering the Nonlinear Least Squares Curve Fitting Session

To enter the nonlinear least squares curve fitting session, select **Analysis:Non-linear Curve Fit:Advanced Fitting Tool** when either the graph or worksheet window is active.

Two NLSF Modes: Basic and Advanced

To help you master the power of Origin's nonlinear least squares fitter, two NLSF modes are available: Basic and Advanced. While both modes allow you to fit your data, they differ substantially in the options they provide as well as in the degree of complexity they entail.

The Basic mode is much simpler to use and understand. Use this mode to:

1) Select a function from a reduced set of built-in functions.

2) Select data sets for fitting.

3) Perform an iterative fitting procedure.

4) Display the results on the graph.

The Advanced mode includes more options. Use this mode to:

1) Define a LabTalk script or Origin C code to initialize parameters.

2) Impose linear constraints.

3) Define your own fitting functions.

4) Specify a weighting method and termination criteria.

5) Display confidence and prediction bands, residue plot, parameter worksheet, and the variance-covariance matrix.

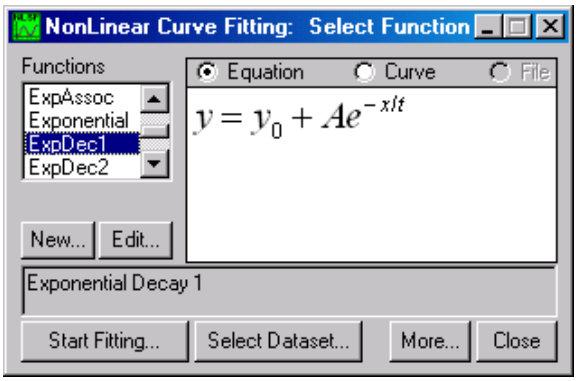
6) Fit multiple data sets with a choice of shared parameters.

7) Change parameter names.

Using the Fitter in the Basic Mode: Examples

By default, when you select **Analysis:Non-linear Curve Fit:Advanced Fitting Tool** from the menu when a graph or a worksheet window is active, Origin's nonlinear least squares fitter starts in the basic mode. When the fitter is in the basic mode, it does *not* have its own menu bar. Switch from the basic to the advanced mode at any time by clicking on the More button.

Fitting a First Order Exponential Decay Function using the Fitter's Basic Mode



Opening a Project File

1) Click the Open button on the Standard toolbar to open the Open dialog box. Select 'Project (*.OPJ)' from the Files of Type drop-down list.

2) In the Origin TUTORIAL folder, double-click on FITEXMP1.OPJ in the list of files. This action opens the Fitexmp1 project with a Graph1 window displaying sample data.

Starting the Basic Mode of the NLSF

1) With the graph window active, select **Analysis:Non-linear Curve Fit:Advanced Fitting Tool**. This menu command opens the Select Function dialog box of the NLSF. If the advanced mode is displayed instead, select **Options:Basic Mode** from the fitter's menu to display the basic mode.

Selecting a Function

1) If the Select Function dialog box is not displayed, click Select Function to display it.

2) In the Functions list box, click on ExpDecay1 to select the First Order Exponential Decay function.

Starting the Fitting

1) Click Start Fitting. An Attention message opens informing you that you have not selected a data set for fitting. You can choose to fit either the current active data set (**data1_b**) or select another data set. Select the active data set. The Fitting Session dialog box replaces the Select Function dialog box.

Fixing Parameters

Suppose that you want to fit the data to the exponential decay function but with a *fixed* value of the vertical offset y0 (=4).

1) Type **4** in the Value text box for the y0 parameter. Clear the Vary check box for this parameter.

2) Type **0.01** in the Value text box for the x0 parameter. Leave the Vary check box selected.

3) Type **8** in the Value text box for the A1 parameter. Leave the Vary check box selected.

4) Type **8** in the Value text box for the t1 parameter. Leave the Vary check box selected.

Performing Iterations

1) Click 1 Iter to perform one iteration. New values of the parameters x0, A1, and t1 are displayed together with the current value of the reduced chi^2. Notice that the parameter value of y0, which we fixed in the previous step, remains unchanged. The theoretical curve corresponding to the current parameter values is displayed in Graph1.

2) Click 100 Iter to perform (at most) 100 iterations. Notice the improvement of the fit.

Finishing Fitting

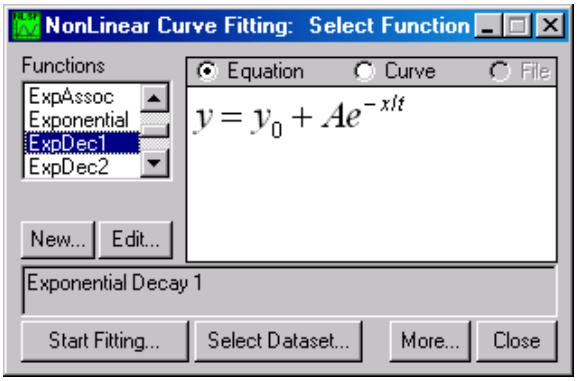
1) Click Done. The fitter's dialog box closes. The parameter values are pasted to the graph.

The Dialog Boxes of the Basic Mode

The basic mode includes five dialog boxes: the Select Function, Define New Function, Edit Function, Select Dataset, and Fitting Session dialog boxes. Open any of these dialog boxes by clicking on the corresponding buttons within the active dialog box.

Basic Mode: The Select Function Dialog Box

By default, this dialog box is displayed when you invoke the curve fitter. You can also access it from the remaining two basic mode dialog boxes by clicking on the Select Function button.



The Functions List Box

This list box provides the list of fitting functions available in the basic mode. In addition to a set of built-in functions, all user-defined functions are displayed. Select a function by clicking on its name.

The View Box

If you have selected a built-in function, the view box to the right of the Functions list box displays either the function's definition (equation) or a curve which shows the function's profile. Switch between the two by selecting the corresponding radio buttons at the top of the view box. If you have selected a function which you had previously defined, then the view box contains the definition of the function.

The Start Fitting and Select Dataset Buttons

Click these buttons to open the Fitting Session and Select Dataset dialog boxes, respectively.

The More Button

Click this button to switch from the basic to the advanced mode.

The New Button

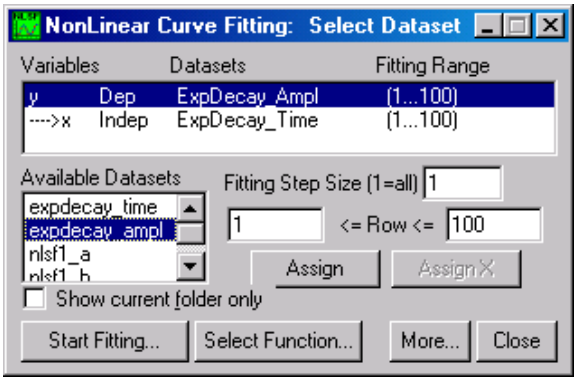
Click this button to open the Define New Function dialog box.

The Edit Button

Click this button to open the Edit Function dialog box.

Basic Mode: The Select Dataset Dialog Box

Edit the Select Dataset dialog box to select the data sets for fitting.



The Variables:Datasets List Box

Each line in this list box includes the following information:

VariableName, Indep. or Depend., *DatasetAssignment*, *Range*

VariableName is the name of the variable. Indep or Depend specifies whether the variable is independent or dependent. *DatasetAssignment* is the name of the data set to which the variable is assigned. *Range* is the data set range used in fitting.

If no data set assignment has been made, the associated section of the line displays question marks. This field updates during data set assignment.

The Available Datasets List Box

This list box displays the names of all the data sets in the project.

The Assign/Assign X Buttons

You must assign all the variables to data sets.

The way in which you assign variables to data sets differs depending on whether you are assigning a dependent or an independent variable.

To assign dependent variables to data sets:

1) Click on the dependent variable you want to assign in the Variables:Datasets list box. The row becomes highlighted. Additionally, the Assign X button becomes unavailable.

2) Click on the data set name you want the variable assigned to in the Available Datasets list box. The data set becomes highlighted.

3) Click Assign to assign the variable to the data set.

To assign independent variables to data sets:

1) Click on the independent variable you want to assign in the Variables:Datasets list box. The Assign X button becomes available.

2) Click on a data set name in the Available Datasets list box.

3) There are now two options. If you want the variable assigned to the data set which you highlighted in step b, click Assign. If you want the variable assigned to the 'x of' the data set which you highlighted in step b (rather than to the data set itself), click Assign X. The 'x of' a data set may have three different meanings: another data set; the data sets associated row numbers, or a defined starting value and a step increment.

Fitting Step Size Text Box

Specify whether you want to skip some points in fitting in this text box. For example, type **3** to use every third point in the data set. Type **1** to use all the data points.

The <= and <= Text Boxes

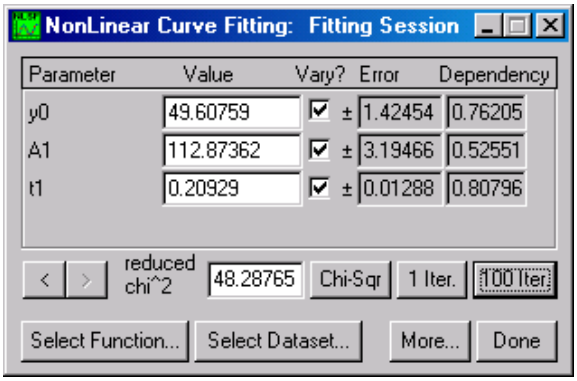
If a dependent variable is highlighted in the Variables:Datasets list box, use '<= Row <=' text boxes to specify the *interval of data set rows* to be used in fitting.

If an independent variable is highlighted in the Variables:Datasets list box, then the space between the two '<=' signs turns into a button. You can toggle the words 'Row' or '<*name of variable*>' on this button. If Row is selected, the meaning is the same as for dependent variables. If the name of the independent

variable is displayed on the button, specify the *interval in units of the independent variable* to be used for fitting. For example, if you have specified **3.1<=x<=9.7**, this means that only the points with the value of the independent variable X between 3.1 and 9.7 will be used in fitting.

Basic Mode: The Fitting Session Dialog Box

Access this dialog box by clicking the Start Fitting button from the other two dialog boxes in the basic mode.



The Parameter Value Text Boxes

These text boxes list the fitting parameters and their current values. Use them to specify what parameter values you want the iterative procedure to start from. Additionally, change the parameter values at any time to enable the iterations to proceed from these new values.

The Vary Check Boxes

Each parameter contains a Vary check box. Select this check box to vary the parameter value during the iterative procedure. Otherwise, the parameter remains fixed at its current value.

The Error List Boxes

If at least one iteration has been done, these list boxes contain the estimates of the standard errors.

The Dependency List Boxes

These list boxes display the parameter dependency. If the equation is overparameterized, there will be mutual dependency between parameters. If this value is close to one, there is strong dependency.

The Chi-Sqr Button

Click Chi-Sqr to display the reduced chi^2 value for the current parameter values. The display of this value is automatically updated after each iteration. You may use this button if you have manually changed some parameter values and want to know what the value is before proceeding.

The 1 Iteration Button

Click 1 Iter to perform one iteration. The new parameter values are displayed in the Parameter Value text box, together with the error and dependency values.

The n *Iterations Button*

Click *n* Iter to cause the fitter to perform, at most, *n* iterations. The number *n* can be changed in the advanced mode. The fitter may perform less than *n* iterations if it detects that further iterations will not improve the fit. Stop the iterations at any time by pressing the ESC key.

The < and > Buttons

These buttons enable you to retrieve the values of parameters which the fitter has already gone through. For example, click the < button to display the parameter values that were current before the last iterations.

Using the Fitter in the Advanced Mode

Access the advanced mode from the basic mode by clicking on the More button.

Some General Notes on the Advanced Mode of the Nonlinear Least Squares Curve Fitter

The fitting menu bar includes five menus: Category, **Function**, **Action**, **Options**, and **Scripts**. Each of these menus contain several commands. In most cases, when a menu command is selected, the dialog box associated with the menu command is displayed in the fitting window. In addition, a fitting toolbar containing twelve buttons displays below the menu bar. Each button is associated with a menu command and can be clicked on to open the respective dialog box. You can toggle the toolbar on and off by (de)selecting **Options:Toolbar** from the fitter's menu.

Menu commands (and the corresponding toolbar buttons) may be temporarily disabled. For example, you cannot select the **Action:Fit** menu command unless you have already selected or defined a fitting function.

The menu command corresponding to the dialog box currently displayed in the fitting window is checked.

The fitting dialog boxes contain buttons, text boxes, drop-down lists, check boxes, and list boxes. Settings in one dialog box often reflect settings in other dialog boxes. For example, you can initialize parameters in the Initializations dialog box. If you then select Action:Fit, the parameter values displayed in the Fitting Session dialog box reflect those set in the Initializations dialog box.

An Example Defining your own Function of Two Variables in the Advanced Mode

This tutorial teaches you how to define your own function of *two* variables to fit sample data sets using the advanced mode of Origin's NLSF. You will write and compile your function using Origin C. The function to be defined is:

act = vm * substr / (km + (1 + inhib / k) * substr)

Opening a Project File

1) Click the Open button on the Standard toolbar to open the Open dialog box. Select 'Project (*.OPJ)' from the Files of Type drop-down list.

2) In the Origin TUTORIAL folder, double-click on FITEXMP3.OPJ in the list of files. This opens the Fitexmp3 project with the Graph1 window displaying sample data.

Starting the Fitter

1) Select **Analysis:Non-linear Curve Fit:Advanced Fitting Tool** to open the NLSF window.

2) If the basic mode of the fitter is displayed, click More to proceed to the advanced mode.

Defining a Function

1) Select **Function:New** from the fitter's menu. This menu command opens the Define New Function dialog box.

2) Type **Tutorial** in the Name text box.

3) Select the User Defined Param. Names check box to enable arbitrary parameter names.

4) Type the following in the Parameter Names text box: **ki,km,vm**. Origin will fit these parameters during the fitting session.

5) Type **substr**,**inhib** in the Independent Var text box. You must use these names for the independent variables when entering the function definition.

6) Type **act** in the Dependent Var text box. You must use this name for the dependent variable when entering the function definition.

7) Define your function in the Definition edit box:

```
double mix = inhib / ki;

act = vm * substr / (km + (1 + mix) * substr);
```

Note: C-language syntax requires that you declare variables prior to use. In this case, we use the statement "**double mix = inhib / ki;**" to both declare and define the variable "mix." The other variables and the parameters in these two equations are declared automatically because we typed them into the **Parameter Names**, **Independent Vars.** and **Dependent Vars.** text boxes in the **Edit Function** dialog box.

8) Verify that the **Use Origin C** check box is selected.

9) From the NLSF menu, select **Scripts:After Fit**. In the **Fit Curve** group, select **Same X as Fitting Data** (this is necessary because the x variable is not a continuous variable).

10) Verify that the **Generate Fit Curve** and **Paste Parameters to Plot** check boxes are selected.

11) From the NLSF menu, select **Function:Save.** This saves the function along with our settings, for future use.

Assigning Variables to Data Sets

1) Select **Action:Dataset** from the fitter's menu. This menu command opens the Select Dataset dialog box.

2) In the Variables:Datasets list box, click on the Act dependent variable to highlight it.

3) In the Available Datasets list box, click on **data1_activity** to highlight it.

4) Click Assign to assign the dependent variable Act to the data set **data1_activity**.

5) In the Variables:Datasets list box, click on the Substr independent variable to highlight it.

6) In the Available Datasets list box, click on **data1_substrate** to highlight it.

7) Click Assign to assign the independent variable Substr to the data set **data1_ substrate**.

8) In the Variables:Datasets list box, click on the Inhib independent variable to highlight it.

9) In the Available Datasets list box, click on **data1_inhibitor** to highlight it.

10) Click Assign to assign the independent variable Inhib to the data set **data1_inhibitor**.

Entering a Fitting Session

1) Select **Action:Fit** from the fitter's menu. This menu command opens the Fitting Session dialog box. Note that selecting **Action: Fit** caused Origin to compile your user-defined fitting function.

Initializing the Parameters

1) Type **0.01** in the Value text box for the parameter ki.

2) Type **1** in the Value text box for the parameter km.

3) Type **100** in the Value text box for the parameter vm.

4) To enable all three parameters to vary during fitting, make sure that the Vary check boxes are all selected.

Fitting the Data

1) Click 100 Iter. The actual number of iterations performed is likely to be less than 100 because a satisfactory fit can be reached with fewer than 100 iterations. You can convince yourself that this is the case by clicking on the 1 Iter button to perform one more iteration. If you do that, the reduced chi^2 value does not change.

Pasting the Parameter Values to the Graph and Exiting the Fitter

1) Click Done.

An Example Fitting Multiple Data Sets to a Function in the Advanced Mode

This tutorial teaches you how to fit multiple data sets to a function using the advanced mode of the NLSF. The function used is Gaussian:

y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2) .

Opening a Project File

1) Click the Open button on the Standard toolbar to open the Open dialog box. Select 'Project (*.OPJ)' from the Files of Type drop-down list.

2) In the Origin TUTORIAL folder, double-click on FITEXMP4.OPJ in the list of files. This opens the Fitexmp4 project with the Graph1 window displaying sample data.

Starting the Fitter

1) Select **Analysis:Non-linear Curve Fit:Advanced Fitting Tool** to open the NLSF window.

2) If the basic mode of the fitter is displayed, click More to proceed to the advanced mode.

Selecting a Function

1) Select **Function:Select** to open the Select Function dialog box.

2) Click on Origin Basic Functions in the Categories list box.

3) Click on Gauss in the Functions list box. This action selects a Gaussian function.

Selecting Multiple Data Sets

1) Select **Action:Dataset** to open the Select Dataset dialog box.

2) Select the Fit Multiple Datasets check box.

3) Click *twice* on the Add Data button to indicate that you want to fit simultaneously *three* data sets to the same function.

4) Click on the x(1) independent variable in the Datasets:Variables list box at the top of the dialog box to highlight it.

5) Click on the **data1_a** data set name in the Available Datasets list box to highlight it.

6) Click Assign to assign the independent variable x(1) to the **data1_a** data set.

7) Repeat the same procedure with the independent variables x(2) and x(3) to assign them to the same **data1_a** data set.

8) Click on the y(1) dependent variable in the Datasets:Variables list box at the top of the dialog box to highlight it.

9) Click on the **data1_b** data set name in the Available Datasets list box to highlight it.

10) Click Assign to assign the dependent variable y(1) to the **data1_b** data set.

11) Repeat the analogous procedure for the dependent variable y(2) to assign it to the **data1_c** data set and for the dependent variable y(3) to assign it to the **data1_d** data set.

Specifying Parameter Sharing

1) Double-click on the w and A parameters in the Parameter Sharing list box to tag them as shared. This causes only one "version" of each of these two parameters to be used for all three data sets, whereas each data set will have its own "version" of the remaining two parameters.

Fitting the Data

1) Select **Action:Fit** to open the Fitting Session dialog box.

2) Leave the initial parameter estimates as they are. Note that for built-in fitting functions, Origin calculates data set specific parameter estimates. This is done automatically when you choose **Action: Fit** from the NLSF menu.

Note also that only one value is listed for w and A parameters because we chose to share those parameter values among the three data sets.

3) Make sure that all the parameters have their Vary check boxes selected to allow them to vary during fitting.

4) Click 100 Iter.

Pasting the Results to the Graph and Exiting the NLSF

1) Click Done.

To Expedite Future Fitting Sessions using the Same Fitting Function and Similar Data

Note that the NLSF will remember which fitting function was last used.

1) Make the worksheet that contains the fitting data sets active.

2) Highlight the data sets that you want to fit.

3) Select **Analysis: Non-linear Curve Fit: Advanced Fitting Tool** . The fitting function is selected and the data sets are assigned automatically. When you select **Action: Fit** the parameters are automatically initialized. You can now start fitting.

Before you Start: The Chi-Square Minimization

Two building blocks of any fitting procedure are:

1) The data which represent the results of some measurements in which one or several *independent* (input) variables ($x_1, x_2, x_3, \cdots$) were varied over a certain range in a controllable manner so as to produce the measured *dependent* (output) variable(s) $y_1, y_2, y_3, \cdots$.

2) The mathematical expression (a function or a set thereof) in the form

$y_1 = f_1(x_1, x_2, x_3, \ldots; p_1, p_2, p_3, \ldots)$ $y_2 = f_2(x_1, x_2, x_3, \ldots; p_1, p_2, p_3, \ldots)$

$y_3 = f_3(x_1, x_2, x_3, \ldots; p_1, p_2, p_3, \ldots)$ which represents the theoretical model believed to explain the

process that produced the experimental data. The model usually depends on one or more parameters $p_1, p_2, p_3, \cdots$.

The aim of the fitting procedure is to find those values of the parameters which best describe the data. The standard way of defining the best fit is to choose the parameters so that the sum of the squares of the deviations of the theoretical curve(s) from the experimental points for a range of independent variables:

$$\chi^2(p_1, p_2, \ldots) = \frac{1}{n^{eff} - p} \sum_i \sum_j w_{ji} \left[y_{ji} - f_j(x_{1i}, x_{2i}, \ldots; p_1, p_2, \ldots) \right]^2$$

is at its minimum. Here, y_{ji} are the measured values of the dependent (output) variable y_j for the values of the independent (input) variables $x_1 = x_{1i}$, $x_2 = x_{2i}$, ...; n^{eff} is the total number of experimental points used in the fitting, and p is the total number of adjustable parameters used in the fitting (the difference $d = n^{eff} - p$ is usually referred to as the number of degrees of freedom). The quantities w_{ji} represent the weights of each experimental point. Four different weighting methods are supported by Origin:

No weight: $w_{ji} = 1$.

Instrumental weights: $w_{ji} = 1/\sigma_{ji}^2$, where σ_{ji} are the error bar sizes stored in error bar columns.

Statistical: $w_{ji} = 1/y_{ji}$.

Any data set: The weights are determined by any user-specified data set so that $w_{ji} = 1/c_{ji}^2$, where c_{ji} are the values of arbitrary data sets.

Direct: $w_{ji} = c_{ji}$

In case there is only one independent and one dependent variable:

$$y = f(x; p_1, p_2, p_3, \ldots)$$

the expression for χ^2 simplifies to:

$$\chi^2(p_1, p_2, \ldots) = \frac{1}{n^{eff} - p} \sum_i w_i \left[y_i - f(x_i; p_1, p_2, \ldots) \right]^2$$

The LM algorithm, starting from some initial parameter values, minimizes $\chi^2(p_1, p_2, \ldots)$ by performing a series of iterations on the parameter values and computing $\chi^2(p_1, p_2, \ldots)$ at each stage. In order to do that, Origin internally calculates partial derivatives $\mathbf{f}'_j = \left[\partial f_j / \partial p_1, \partial f_j / \partial p_2, \ldots, \partial f_j / \partial p_p \right]$ for all the values of the input variables. For built-in functions, all the derivatives are computed using analytic

expressions. For user-defined functions, the partial derivatives are computed numerically. The computation is thus faster for built-in functions than for user-defined functions. (Note: You can define a user-defined function with partial derivatives.)

You can limit the set of the allowed values which the fitting parameters can take during the iterative procedure by imposing linear constraints. Origin internally implements the constraints by means of the Lagrange multiplier method.

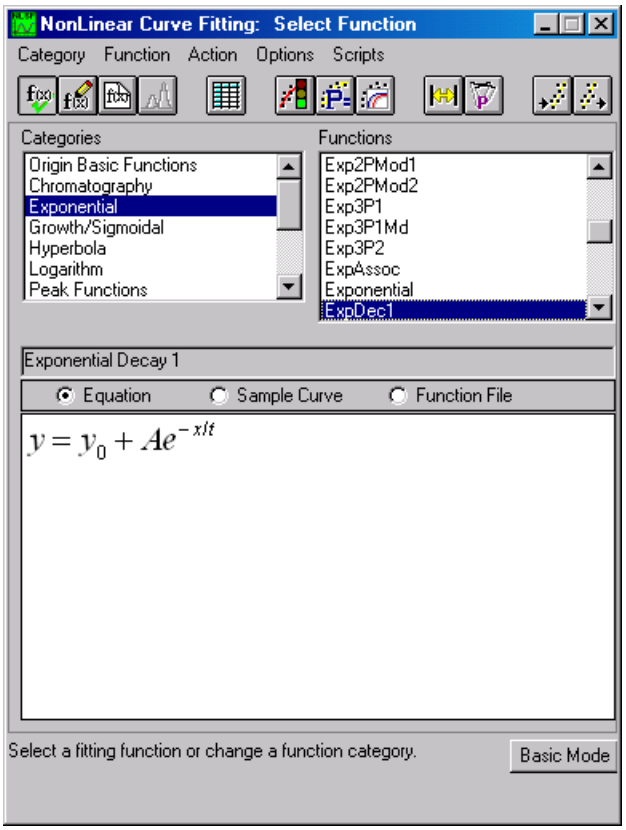
Note: The NLSF always reports the reduced chi^2 value, not chi^2. In some locations of the NLSF, reduced chi^2 is labeled "chi^2". In other locations, it is labeled "chi^2/DoF". In all cases the actual value is reduced chi^2.

Selecting an Existing Fitting Function

Select **Function:Select** to select a built-in or previously saved user-defined function for fitting. This menu command opens the Select Function dialog box.

Note: To learn more about fitting with a built-in function, review the NLSF BUILT IN FUNC.OPJ project located in your Origin \SAMPLES\ANALYSIS\CURVE FITTING folder.

The Select Function Dialog Box



The Categories List Box

Select the desired category in this list box. Origin provides a variety of built-in functions. Functions are grouped into several categories based on the area of primary use.

The Functions List Box

Functions belonging to the selected category are displayed in this list box. The listed functions include both built-in and user-created functions. Click to select the desired function.

Select **Function:Add** to add a function to the selected category.

Select **Function:Delete** to remove the highlighted function from the list.

The Equation Radio Button

Select the Equation radio button to display the function in the lower view box. The radio button is unavailable if a user-defined function is selected.

The Sample Curve Radio Button

Select the Sample Curve radio button to display a sample curve of the currently selected function. The curve is displayed in the lower view box. The radio button is unavailable if a user-defined function is selected.

The Function File Radio Button

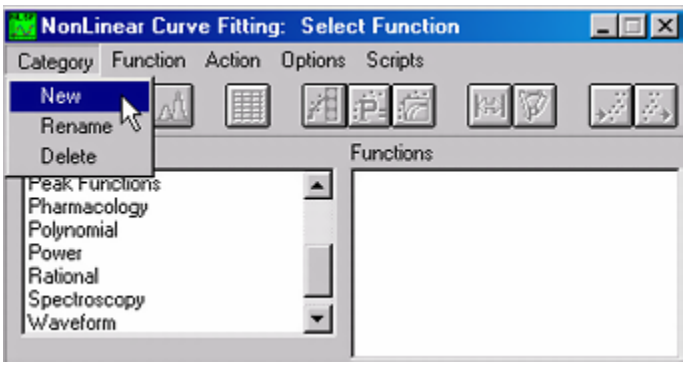
Select the Function File radio button to display the function definition file associated with the function. The function definition file contains all the information about the function and the current fitting session. *It is not necessary to view this file.* In fact, most of the contents of this file can be changed using other dialog boxes.

User-Defined Fitting Functions

This section discusses creating user-defined fitting functions with the Nonlinear Least Squares Fitter (NLSF) Advanced Fitting Tool. Once a function is defined in the NLSF and added to an NLSF fit category, the function becomes available from the Fitting Wizard.

Adding a new Category

New functions can be added to existing categories, or they can be added to a new category. To create a new category before defining a new fitting function.

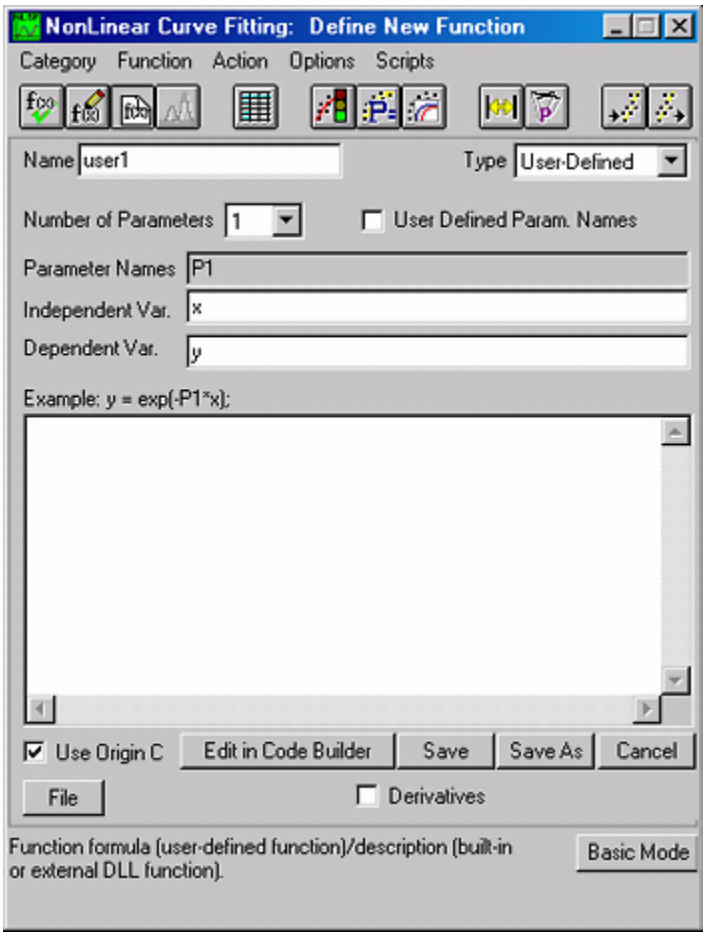


1) From the Origin program menu, select Analysis:Nonlinear Curve Fit:Advanced Fitting Tool.
2) From the NLSF menu, select **Category:New**.
3) In the Category Name text box, type ***Category Name*** (spaces are permissible) and click **OK**.

Defining a New Function

To define a new function, choose **Function:New** from the NLSF menu.

The Define New Function Dialog Box



The Name Text Box

The Name text box will display a default name, such as user1. Enter the name of your function.

Note: The function name *must not contain spaces or special characters*. Failure to adhere to function naming conventions will generate a warning.

When you save a user-defined function, it is stored in the Origin\FitFunc folder as *FunctionName*.FDF.

The Type Drop-Down List

The Type drop-down list offers two choices: **User-Defined** and **External DLL**. The default type – the appropriate choice in most cases – is User-Defined.

The External DLL option gives the user access to a function that is coded and compiled using a non-native compiler (such as a C or Fortran compiler). This method pre-dates Origin C and, as such, is now less compelling. However, OriginPro customers will find documentation of this method in Section 7.3 (page 340) of the OriginPro manual.

The Number of Parameters Drop-Down List

By default, Origin assigns names of P1, P2 , etc., to function parameters. For example, setting the Number of Parameters drop-down to 3, generates the parameter names of P1, P2, and P3.

If you opt for user-defined parameter names, it is *not* necessary to set the Number of Parameters drop-down list.

The User Defined Param. Names Check Box.

This check box must be selected if you specify your own parameter names.

The Parameter Names Text Box

If default parameter names are used, this text box is not editable. It is only editable when the User Defined Param. Names checkbox is selected.

Note: *The following user defined parameter and variable names are not allowed:* x1, x2,….x*n*, y1, y2,…y*n*, z1, z2,…z*n*, and the letter i. The letters t, j, and e should also be avoided. Furthermore, there are some system variables that should be avoided. For more information on these system variables, consult the LabTalk Help file by choosing **Help:Programming:LabTalk Reference** from the Origin menu. You are strongly encouraged to *choose parameter and variable names that contain more than one character*. If you use a name that is not allowed, you will be prompted to change it when you start fitting.

The Independent Var. Text Box

Specify the name(s) of the independent variable(s), using comma separators as needed. Note that the NLSF allows more than one independent variable.

See the note above concerning parameter and variable names.

The Dependent Var. Text Box

Specify the name(s) of the dependent variable(s), using comma separators as needed. Note that NLSF allows more than one dependent variable.

See the note above concerning parameter and variable names.

The Definitions Text Box

The function definition is typed into this text box. If you define your function using Origin C (the Use Origin C box is check box is selected), it may be more convenient to use the Code Builder workspace to type your function. Refer to the Edit in Code Builder Button section below for more details. Once you have defined your function in Code Builder, you can do further editing in the Definitions text box.

If the Use Origin C check box is *cleared*, you must type the function in the Definitions text box. This applies to all forms (Expressions, Y-Script, or Equations) available from the Form drop-down list.

The Use Origin C Check Box

When defining a new function, the NLSF default setting is to use Origin C, Origin's ANSI C-compatible programming language. This option offers the most speed and flexibility for defining your function.

When the Use Origin C check box is selected, the Form drop-down list is unavailable.

The Form Drop-down List

The available function forms are Expression, Y-Script, and Equations.

Note: When the Use Origin C check box is selected, the Form drop-down list is unavailable. In actuality, both Y-Script and Equations forms will work with Origin C. Only the Expression form is incompatible.

- Expression. Use is limited to function definitions with a single dependent variable. The function definition follows the form of this example:

  ```
  a*x+b*x^2+exp(c*x)
  ```

- Y-Script. Use this form when using LabTalk script to define your function. Each dependent variable must be defined in the script using the form…

  ```
  y =…
  ```

  where y is the dependent variable.

- Equations. This option is appropriate for one or more dependent variables. Define your function in Definitions text box. For multiple dependent variables, type a separate line for each following the form of this example

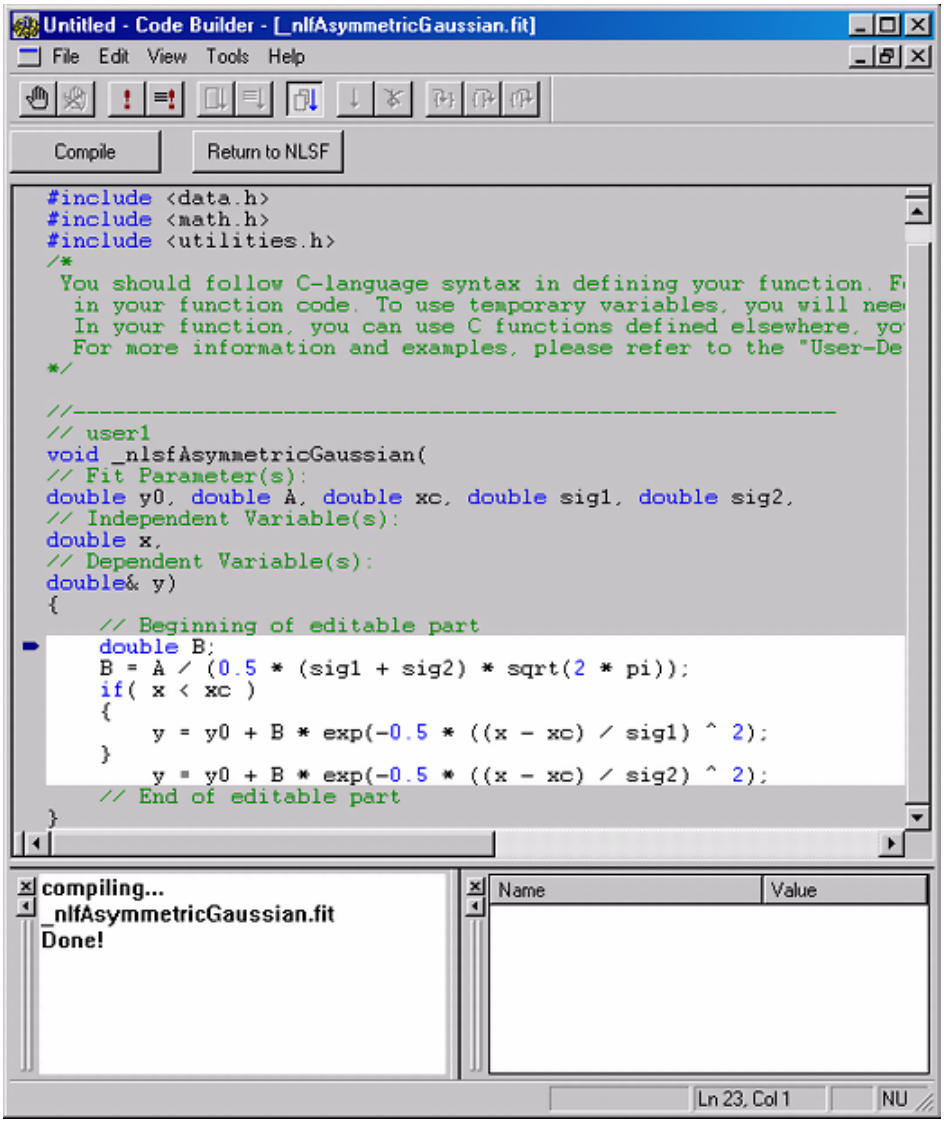
  ```
  y1 = ….
  y2 = ….
  ```

  where `y1` and `y2` are dependent variables. Do not include any loops or `if-else` clauses. Temporary variables are permissible.

Note: If your function definition uses constants and the constant values are not specified in the function definition itself, they must be assigned in the Constants text box of the Initialization dialog box (choose **Scripts:Parameter Initialization** from the NLSF menu).

The Edit in Code Builder Button

This button is available when Use Origin C is enabled. Clicking this button opens a specialized version of the Code Builder workspace. This specialized view will open with an active window named _nlf*FunctionName*.fit (_nlfAsymmetricGaussian.fit, in this example). This is the edit window for the new function definition.


Untitled - Code Builder - [_nlfAsymmetricGaussian.fit]
File Edit View Tools Help
Compile
Return to NLSF
#include <data.h>
#include <math.h>
#include <utilities.h>
/*
You should follow C-language syntax in defining your function. F
in your function code. To use temporary variables, you will nee
In your function, you can use C functions defined elsewhere, yo
For more information and examples, please refer to the "User-De
*/
//---
// user1
void _nlsfAsymmetricGaussian(
// Fit Parameter(s):
double y0, double A, double xc, double sig1, double sig2,
// Independent Variable(s):
double x,
// Dependent Variable(s):
double& y)
{
// Beginning of editable part
double B;
B = A / (0.5 * (sig1 + sig2) * sqrt(2 * pi));
if(x < xc)
{
y = y0 + B * exp(-0.5 * ((x - xc) / sig1) ^ 2);
}
y = y0 + B * exp(-0.5 * ((x - xc) / sig2) ^ 2);
// End of editable part
}
compiling...
_nlfAsymmetricGaussian.fit
Done!
Name
Value
Ln 23, Col 1
NU

The first few lines of code are `#include` statements that identify various header files required for compiling the fitting function. The actual function definition begins with the statement:

`void _nlsfAsymmetricGaussian(…`

The parameters, independent variables, and dependent variables are declared at the beginning of this function definition. After these declarations, there is an editable section – the area bounded in white – that is reserved for entering your function definition.

The above figure shows the definition of the asymmetric Gaussian function having been typed in. Note that the function definition must comply with C programming language syntax. For instance, *the*

parameters and all variable types are case sensitive. Intermediate variables – such as `B` in this example – *must be declared first* using a statement such as:

```
double B;
```

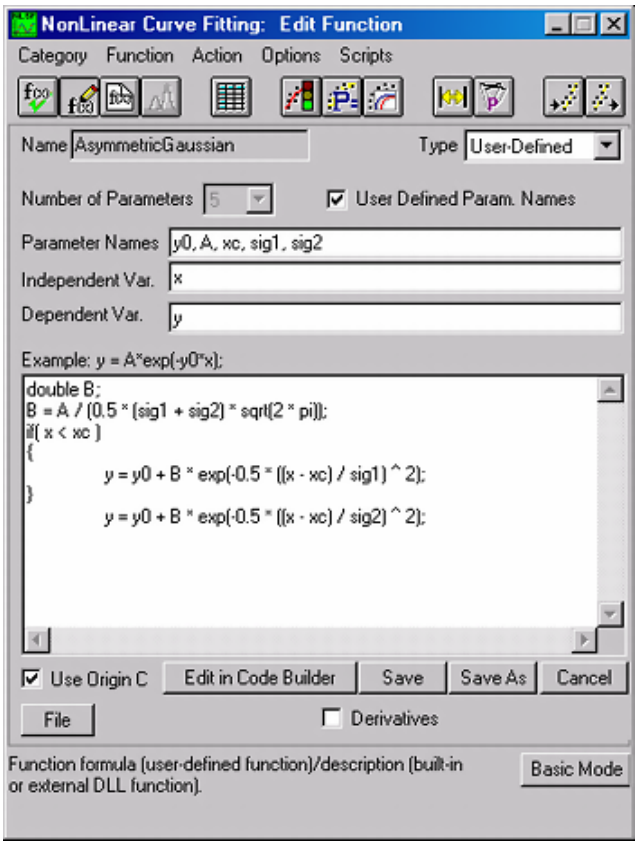
This declaration must occur before the variable is used in the function definition.

Note that the function is of type `void`, which means that no values are returned by the function. Instead, the dependent variable value is set inside the function code. In our example, the dependent variable y is assigned a different value, dependent upon whether x is less than or greater than the centroid parameter, xc.

Once the function is defined, you must verify that your syntax is correct. To test, click the Compile button at the top of the Code Builder workspace. This action compiles the function code using Origin C. Any errors generated in the compiling process are reported in the Code Builder output window at the bottom of the workspace. This window also reports when a file has successfully compiled (see the above figure).

Once the function has been defined and compiled, you can return to the NLSF interface by clicking the Return to NLSF button at the top of the window. This closes the specialized Code Builder window.

As mentioned, you can do further editing of your function directly in the NLSF Function Definition text box. You can also click the Edit in Code Builder button and return to the Code Builder workspace to edit your function.


NonLinear Curve Fitting: Edit Function
Category Function Action Options Scripts
Name AsymmetricGaussian
Type User-Defined
Number of Parameters 5
User Defined Param. Names
Parameter Names y0, A, xc, sig1, sig2
Independent Var. x
Dependent Var. y
Example: y = A*exp(-y0*x);
double B;
B = A / (0.5 * (sig1 + sig2) * sqrt(2 * pi));
if(x < xc)
{
y = y0 + B * exp(-0.5 * ((x - xc) / sig1) ^ 2);
}
y = y0 + B * exp(-0.5 * ((x - xc) / sig2) ^ 2);
Use Origin C
Edit in Code Builder
Save
Save As
Cancel
File
Derivatives
Function formula (user-defined function)/description (built-in or external DLL function).
Basic Mode

Note 1: It is not necessary to close Code Builder to return to the NLSF. You can leave the Code Builder workspace open and switch between the NLSF and Code Builder. However, if you leave Code Builder open, you will not be able to edit to your function from the NLSF; the NLSF Function Definition text box will not be editable. Furthermore, if you make changes to your function in the Code Builder workspace, you should click the Compile Button so that when you switch to the NLSF, your function is updated. We recommended that you click the Return to NLSF button to close Code Builder before returning to the NLSF. If you wish to debug the function by setting break points in your code, it makes sense to leave Code Builder open. For further information on debugging, select **Help:Programming:Programming Guide…** from the Origin menu and search on **debug**.

Note 2: If after defining your function in Code Builder you click the Return to NLSF button *without* compiling your function, the function will compile automatically when you select **Action:Fit** from the NLSF menu.

The Save Button

Click the Save button to save the function as *functionName*.FDF. The default folder for storing the function file is the \FitFunc subfolder in the Origin software directory. If a function of the same name already exists, the Save As dialog box opens and the user is asked to give the function a new name. Assigning a new name to the function will update the Name field in the Function Name text box.

Note that once you save the function file, the Function Name text box is no longer editable. To change the name of a saved function, save the function with a different name using the Save As button.

The Save As Button

The Save As button opens the Save As dialog box. The Save As button allows you to save the current function under another name. Note that choosing another name assigns this name to both the function name and the disk (.FDF) file. If a function of the same name already exists, the user is prompted to choose a different name.

The Cancel Button

Click the Cancel button to discard function modifications made since the function file was last saved.

The File Button

Click the File button to display and/or edit the function definition file associated with the function. To return to the Edit page, click on the Form button.

The Derivatives Check Box

Specifying partial derivatives of your function can reduce the time it takes to perform a set of iterations. However, given the much-enhanced speed of fitting achieved with Origin C, specifying partial derivatives may not be necessary.

If you wish to specify partial derivatives, note that you must specify the derivatives of the function of the dependent variable in terms of the fit parameters. Furthermore, partial derivatives with respect to *all* fitting parameters need to be specified.

If you have chosen to define the function using Origin C, the variables for the partial derivatives will be pre-defined in Code Builder. You just need to enter the expression for them..

For example, if the function is:

```
y = P1 + P2 * x + exp(P3 * x)
```

then the variables `dy_P1`, `dy_P2`, and `dy_P3` will be available, and you will need to enter the following equations for the partial derivatives:

```
dy_P1 = 1;
dy_P2 = x;
dy_P3 = x * exp(P3 * x);
```

Note that if you *do not* use Origin C and are defining your function using LabTalk with the Form drop down list set to Y-Script (the only form that is compatible with use of derivatives), then the notation for partial derivatives is different. In this case, the partial derivatives for the above example would be:

```
y'P1 = 1;
y'P2 = x;
y'P3 = x * exp(P3 * x);
```

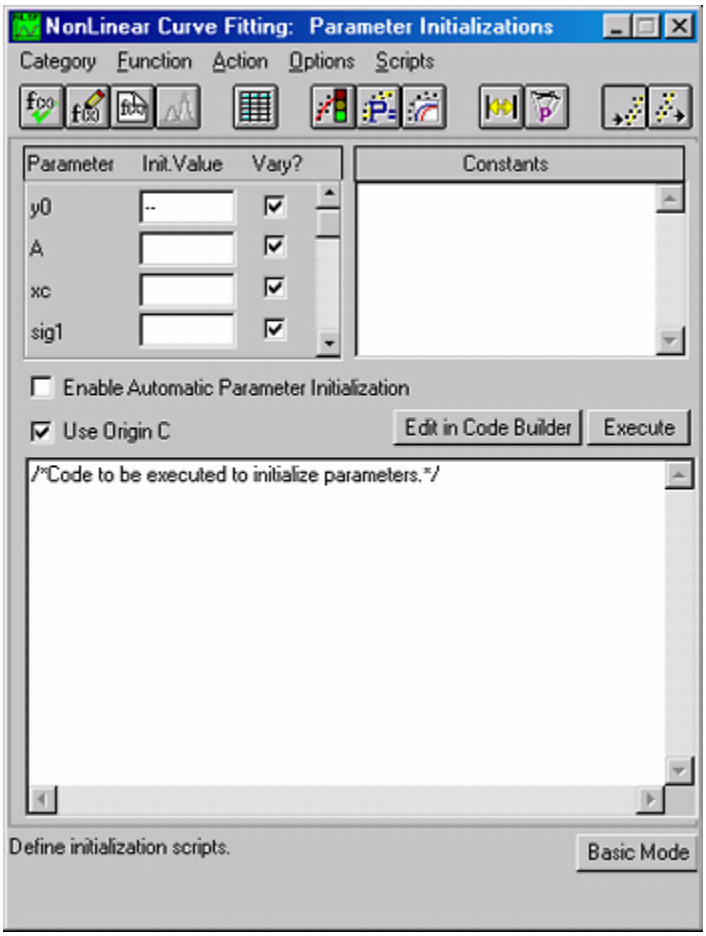
Defining Parameter Initialization Code

Good parameter initialization results in fast and reliable model/data convergence. Automatic parameter initialization can effectively approximate parameter values prior to fitting by generating dataset-specific parameter estimates.

The NLSF provides automatic parameter initialization code for all built-in functions. For user-defined functions, you must add your own parameter initialization code. If no parameter initialization code is provided, then the NLSF registers all parameter values as missing values. If parameter values are missing, you must enter "guesstimate" parameter values to start the iterative fitting process.

To open the parameter initializations dialog, choose **Scripts:Parameter:Initialization** from the NLSF menu.

The Parameter Initializations Dialog Box



The Parameters Group

This group contains the parameter name, an editable text box with current parameter value and a check box control for varying or fixing the parameter value during the iterative fitting process.

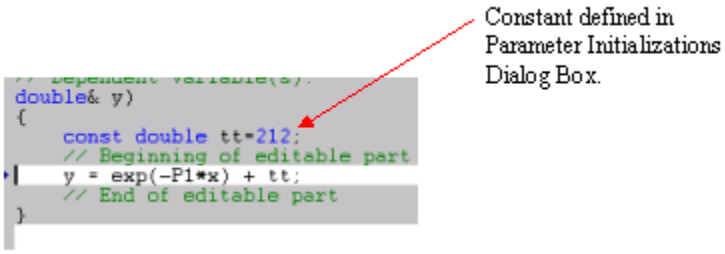
Until the fit dataset is assigned and the automatic parameter initialization code is executed, the parameters will register as missing values. The Vary check box is checked by default.

The Constants Text Box

If your function definition contains constants (not to be confused with parameters and variables), you will need to define those constants in this text box, using this format:

```
constant1 = value1;
constant2 = value2;
```

When using Origin C to define your function, any constant you specify in this text box will appear in the function body when you edit/view the function in Code Builder. You should define your constants in this text box before editing your function in Code Builder. This will ensure that your constants appear in your function definition.



If you are defining your function using LabTalk, with the Form drop-down set to Y-Script, then the constant(s) you specify in this text box will be available for use in your function definition script.

You can also use externally defined constants in your Y-script function (e.g., constants defined in the script window). In such cases, you can use the constant in your function definition script, and later assign values to the constant in the Constants text box.

There same naming restrictions apply to constants as apply to parameter and variable names: x1, x2,….x*n*, y1, y2,…y*n*, z1, z2,…z*n*, and the letter i *are not allowed*. The letters t, j, and e should also be avoided. Furthermore, there are some system variables that should be avoided. For more information on these system variables, consult the LabTalk Help file by choosing **Help:Programming:LabTalk Reference** from the Origin menu. You are strongly encouraged to *choose constant names that contain more than one character.*

The Enable Automatic Parameter Initialization Check Box

This check box determines whether automatic parameter initialization code is executed when you choose **Action:Fit** from the NLSF menu. This setting is saved with each function file. If this check box is *cleared*, then the user needs to click the Execute button to run the initialization code. For new functions, this check box is cleared by default. For built-in functions, this check box is selected by default, but can be cleared at your discretion.

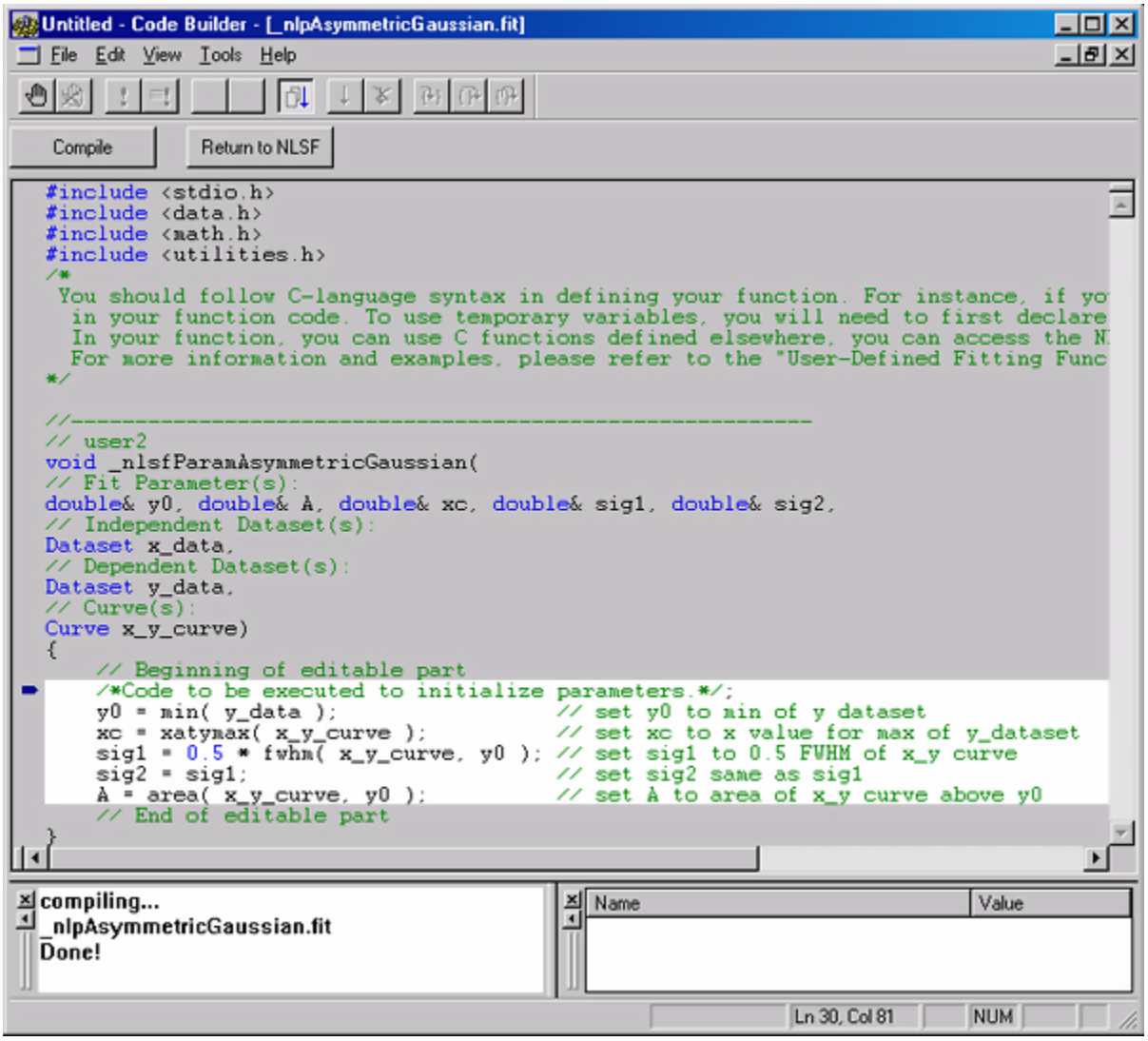
Note: If datsets for fitting are not assigned, the parameter initialization code will fail to execute.

The Use Origin C Check Box

When you create a new function, this check box is selected by default. When this check box is selected, parameter initialization code must be defined using Origin C. If this box is *cleared,* the parameter initialization code is interpreted as LabTalk script. Leaving the check box selected (using Origin C) optimizes parameter initialization.

The Edit In Code Builder Button

This button is available when the user has selected the Use Origin C check box. Clicking the button opens a specialized version of the Code Builder workspace. This workspace will open with an active window named _nlp*functionName*.fit (_nlpAsymmetricGaussian.fit, in this example). This is the edit window for the parameter initialization code.


Untitled - Code Builder - [_nlpAsymmetricGaussian.fit]
File Edit View Tools Help
Compile
Return to NLSF
#include <stdio.h>
#include <data.h>
#include <math.h>
#include <utilities.h>
/*
You should follow C-language syntax in defining your function. For instance, if yo
in your function code. To use temporary variables, you will need to first declare
In your function, you can use C functions defined elsewhere, you can access the N
For more information and examples, please refer to the "User-Defined Fitting Func
*/
//---
// user2
void _nlsfParamAsymmetricGaussian(
// Fit Parameter(s):
double& y0, double& A, double& xc, double& sig1, double& sig2,
// Independent Dataset(s):
Dataset x_data,
// Dependent Dataset(s):
Dataset y_data,
// Curve(s):
Curve x_y_curve)
{
// Beginning of editable part
/*Code to be executed to initialize parameters.*/;
y0 = min(y_data); // set y0 to min of y dataset
xc = xatymax(x_y_curve); // set xc to x value for max of y_dataset
sig1 = 0.5 * fwhm(x_y_curve, y0); // set sig1 to 0.5 FWHM of x_y curve
sig2 = sig1; // set sig2 same as sig1
A = area(x_y_curve, y0); // set A to area of x_y curve above y0
// End of editable part
}
compiling...
_nlpAsymmetricGaussian.fit
Done!
Name
Value
Ln 30, Col 81
NUM

The first few lines of code are `#include` statements that identify various header files required for compiling the initialization code. The initialization function starts with the statement (for this example):

```
void _nlsfParamAsymmetricGaussian(…
```

The parameters, independent variables, and dependent variables are declared at the beginning of this function definition. In addition to these, a few other Origin objects are also declared. A Dataset object is declared for each of the independent and dependent variables. A Curve object is declared for each xy data pair.

```
Dataset x_data,
Dataset y_data,
Curve x_y_curve
```

The Dataset objects point to the x and y datasets for which you are trying to find a best fit. Therefore, the Dataset objects should be used in the initialization code without performing any modifications to them; modifications of the Dataset objects will alter the dataset to be fit.

The Curve object is a copy of the dataset curve that results from pairing an x and a y dataset. You can manipulate this Curve copy in the initialization code without affecting the fit dataset. Many Origin C functions take the Dataset or the Curve as an argument and return potentially useful properties (as, for instance, assigning initial parameter estimates in the initialization code).

Below these declaration statements, there is an editable section – the area bounded in white – that is reserved for entering the initialization code. The above figure shows some parameter initialization code for the asymmetric Gaussian function. Note that the function definition follows the requisite C syntax. Note, also, that the function is of type `void`, which means that our function returns no values. Instead, the parameter variables are stored in the function code. The y0 parameter is initialized using the minimum value of the y dataset, the xc parameter is initialized using the x value that corresponds to the maximum y value (centroid of the peak in the data) etc.

Initialization is accomplished by calling built-in functions that take a dataset or a curve object as an argument. Such functions are prototyped in the data.h header file and the C code for these functions can be found in the file internal.c, in OriginC\System subfolder.

Once the initialization function is defined, you should verify that the syntax is correct. To do this, click the Compile button at the top of the workspace. This compiles the function code using Origin C. Any errors generated in the compile process are reported in the Code Builder Output window at the bottom of the workspace. The Output window reports that the compilation is successful. (see the above image).

Once the initialization code has been defined and compiled, you can return to the NLSF interface by clicking on the Return to NLSF button at the top of the workspace. This will close Code Builder and return you to the NLSF interface. From there, you can do further editing of your code in the Initialization Code text box or you can click the Edit in Code Builder button again to launch Code Builder.

Note: It is not necessary to close Code Builder to return to the NLSF. You can leave the Code Builder workspace open and switch between the NLSF and Code Builder. However, if you leave Code Builder open you will not be able to edit to your code from the NLSF; the Initialization Code text box will not be editable. Furthermore, if you make changes to your code in the Code Builder workspace, you should click the Compile Button so that when you switch to the NLSF, your code is updated. We recommended that you click the Return to NLSF button to close Code Builder, before returning to the NLSF. If you wish to debug your code by setting break points, it makes sense to leave Code Builder open. For further information on debugging, select **Help:Programming:Programming Guide…** from the Origin menu and search on **debug**.

The Execute Button

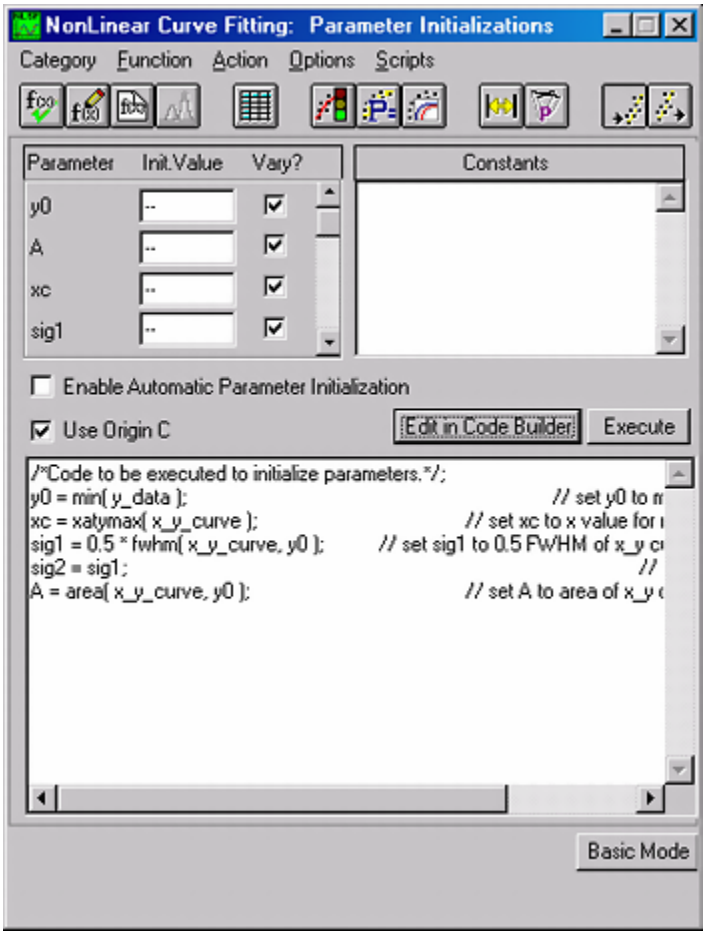
Click the Execute button as needed to execute the parameter initialization code and assign parameter values. Normally, when a function with parameter initialization code is used (and the Enable Automatic Parameter Initialization check box is selected), the initialization code runs automatically when the iterative fitting process begins. The Execute button thus provides a means to reset the parameter values to the initial "guesstimate" values. This is useful if the fit does not converge and the user wants to adjust initial parameter values or fix (prevent from varying) a parameter value. Additionally, you might change the initialization code itself , then click the Execute button to recompute initial parameter values.

Note1: If Automatic Parameters Initialization is enabled, adjustments to parameters will be overwritten when you select **Action:Fit,** unless you have changed the initialization code itself.

Note2: If datsets for fitting are not assigned, the parameter initialization code will fail to execute.

The Initialization Code Text Box

This text box contains the parameter initialization code. The code can be edited in this text box, or it can be edited in Code Builder by clicking on the Edit in Code Builder button. If you make changes to the code in this text box, you can click the Execute button to compile and execute the code. Compilation errors will produce an "Error during compilation" message in the status area at the bottom of the NLSF interface.



Saving the Parameter Initialization Code

When you have defined your parameter initialization code, select **Function:Save** from the NLSF menu. This saves the fitting function with the parameter initialization code, to a fitting function (.FDF) file. You can also save the function using the Save or Save As buttons on the **Function:Edit** page.

Fitting with the User-defined Function

Once you save the user-defined function, you can use it in the same way that you use a built-in curve fitting function. To read more about how to use an existing function, please see Selecting an Existing Fitting Function.

Accessing the NLSF Object and Properties

When you use Origin C to define your fitting function and/or your parameter initialization code, you can access the NLSF object and its properties. For instance, you might use…

```
LabTalk.NLSF.Func$ = "Gaussian";
```

…to set your fit function to Gaussian.

The Origin C `using` statement provides a short cut for accessing the NLSF object properties. Consider this function definition code example:

```
using NLSF = LabTalk.NLSF;
if(NLSF.CurRow < 21)
      y = P1 + P2 * x;
else
      y = P1 + P3 * x^2;
```

In this example, the current row property of the NLSF object is used to fit the first 20 rows of data with one function while the remaining data are fit with another function.

Accessing Other Origin C Functions in your NLSF Code

When you use Origin C to define your fitting function and/or your parameter initialization code, you can access Origin C functions that you have created outside of the NLSF environment. To access these functions, do the following:

1) Add the Origin C function to your Code Builder workspace. For more information, look up index entry "Workspace, adding files" in the Origin 7 Programming Guide (**Help:Programming…:Programming Guide** from the Origin menu).

2) Create a header file that prototypes the function(s) that you want to access.

Add this header file to the nlsf.fit template file in your \OriginC\NLSF subfolder .

This is the method by which the parameter initialization functions are included for use in the NLSF. These functions (min(), yatxmax(), area() etc.) are defined in internal.c and are prototyped in data.h. The data.h header file is included in the nlsf.fit template file and so is included any time you code with Origin C in the NLSF. The internal.c file is a special file that the NLSF loads and adds to your workspace any time you that compile code with Origin C.

Editing the Function

The Edit Function dialog box is only intended for editing *user-defined* functions (for built-in functions, see note below).

Select **Function:Edit** to edit the selected function. This menu command opens the Edit Function dialog box. This menu command is not available if you have not selected or defined a function.

Note: If you want to modify a built-in function, copy the equation in the Description text box (it is selectable, but not editable) to the Clipboard, choose **Function:New** from the NLSF menu and paste the

equation into the new function Description text box. Then you can proceed to modify the equation and save it with a new name.

The Edit Function Dialog Box

The Name Text Box

When editing an existing function, the Name text box is not editable. To change the name of a saved function, save the function with a different name using the Save As button.

The Type Drop-Down List

The function type is selected from the drop-down list. Choose from User-Defined (default) or External DLL.

The Number of Parameters Drop-Down List

Select the number of fitting parameters from this drop-down list. This drop-down list is not available once the user-defined function has been saved with user-defined parameters, though the number of parameters will update if new parameters are added to the Parameter Names text box.

The User Defined Param. Names Check Box

Select this check box to define new names for the function parameters.

The Parameter Names Text Box

The names of the parameters are displayed in this text box. If the User Defined Param. Names check box is selected, you can edit your own parameter names in this text box. Otherwise, the parameter names are set by default to: P1, P2, etc. When entering parameter names in this text box, separate the names by commas.

The number of parameters selected from the Number of Parameters drop-down list must correspond with the number of names in this text box.

Note: If you change the parameter names you must also change the function definition in the Definition text box. Note that t*he following user defined parameter and variable names are not allowed:* x1, x2,….x*n*, y1, y2,…y*n*, z1, z2,…z*n*, and the letter i. The letters t, j, and e should also be avoided. Furthermore, there are some system variables that should be avoided. For more information on these system variables, consult the LabTalk Help file by choosing **Help:Programming:LabTalk Reference** from the Origin menu. You are strongly encouraged to *choose parameter and variable names that contain more than one character*. If you use a name that is not allowed, you will be prompted to change it when you start fitting.

The Independent Var. Text Box

Specify the names of the independent variables in this text box. Separate parameters by commas.

The Dependent Var. Text Box

Specify the names of the dependent variables in this text box. Separate the parameters by commas.

The Description/Definition Text Box

Alter the definition of the function in the Definition text box. To learn about defining your function and compiling it using Origin C, see Defining a New Function.

The Use Origin C Check Box

You can define a fitting function directly in the Definitions text box using Origin C code. To do this, your function must be of the form Y-Script or Equation and the Use Origin C check box must be selected.

If your equation is in the Expression form, it will not be recognizable by Origin C. To use the Origin C compiler, you will have to modify your Description to use the Equation or Y-Script form.

If you choose to select the Use Origin C check box, you can enter your Origin C code in the Definitions text box, or you can use Code Builder, the Origin C development environment, to write or edit your code.. To learn about editing your function in Code Builder and compiling it using Origin C, see Defining a New Function.

If the Use Origin C check box is *not* selected, you must type your function in the Definition text box.

The Form Drop-Down List (user-defined functions only)

Select a form for the user-defined function from the Form drop-down list. The drop-down list includes: Expression, Y-Script, and Equations. Note that if you have written your function to be compiled using Origin C and the Use Origin C check box is selected, the Form drop-down list is not visible. For more information on defining your function so that it is compatible with Origin C, see Defining a New Function.

The File/Form Button

Click File to display (and edit) the function definition file associated with the function.

When the function definition file is displayed in the text box, the Form button is available. Click this button to exit the viewing mode of the function definition file.

The Derivatives Check Box

Specifying partial derivatives of your function can reduce the time it takes to perform a set of iterations. However, given the much-enhanced speed of fitting achieved with Origin C, specifying partial derivatives may not be necessary. For more information on defining your function so that it is compatible with Origin C, see Defining a New Function.

The Save Button

Click Save to save the function modifications in a disk file. The file is named using the text in the Name text box.

The Save As Button

The Save As button opens the Save As dialog box. The Save As button allows you to save the current function under another name. Note that choosing another name assigns this name to both the function

name and the disk (.FDF) file. If a function of the same name already exists, the user is prompted to choose a different name.

The Cancel Button

Click Cancel to discard the function modifications in the Edit Function dialog box.

Selecting the Data Sets

After selecting a model for fitting, you must select the data sets for fitting and assign the function variables to the data sets. Select **Action:Dataset** to open the Select Dataset dialog box. Because the number of both the dependent and the independent variables must be known to perform the data set assignments, you must select or define function(s) *prior to entering* the Select Dataset dialog box.

The Select Dataset Dialog Box

The Variables:Datasets List Box

Each line in this list box includes the following information:

VariableName, Indep. or Depend., *DatasetAssignment*, *Range*

VariableName is the name of the variable. Indep or Depend specifies whether the variable is independent or dependent. *DatasetAssignment* is the name of the data set to which the variable is assigned. *Range* is the data set range used in fitting.

If no data set assignment has been made, the associated section of the line displays question marks. This field updates during data set assignment.

The Available Datasets List Box

This list box displays the names of all the data sets in the project.

The Assign/Assign X Buttons

You must assign all the variables to data sets.

The way in which you assign variables to data sets differs depending on whether you are assigning a dependent or an independent variable.

To assign dependent variables to data sets:

1) Click on the dependent variable you want to assign in the Variables:Datasets list box. The row becomes highlighted. Additionally, the Assign X button becomes unavailable.

2) Click on the data set name you want the variable assigned to in the Available Datasets list box. The data set becomes highlighted.

3) Click Assign to assign the variable to the data set.

To assign independent variables to data sets:

1) Click on the independent variable you want to assign in the Variables:Datasets list box. The Assign X button becomes available.

2) Click on a data set name in the Available Datasets list box.

3) There are now two options. If you want the variable assigned to the data set which you highlighted in step b, click Assign. If you want the variable assigned to the 'x of' the data set which you highlighted in step b (rather than to the data set itself), click Assign X. The 'x of' a data set may have three different meanings: another data set; the data sets associated row numbers, or a defined starting value and a step increment.

The Fit Multiple Datasets Check Box

This check box allows you to fit multiple data sets to the *same* function. This check box, as well as the Add Data and Remove Data buttons, and the Parameter Sharing list box, are not available if your function contains more than one dependent variable.

To fit to multiple data sets:

1) Select the Fit Multiple Datasets check box. The Parameter Sharing list box and the Add Data and Remove Data buttons become available. The Parameter Sharing list box displays all the parameters. If you have not clicked on the Add Data button before, the Variables:Datasets list box still lists all the variables only once.

2) Click Add Data. This action allows you to fit your function to two data sets, which is reflected in the updated Variables:Datasets list box. There are now two entries for each variable, with each entry being indexed, such as, y(1), y(2), x(1), x(2). Each time you click Add Data, you enable one more data set to be fitted. You can remove them one-by-one by clicking on the Remove Data button.

3) Assign the variables to data sets. You *must* assign *all* the variables in the Variables:Datasets list box to data sets.

4) To share a parameter among all the data sets, double-click on one or more parameters in the Parameter Sharing list box. "Shared" is displayed next to the parameter name. If a parameter is not tagged as "Shared", then there will be a separate "version" of the parameter for each data set. If a parameter is tagged as "Shared", there will be only one, common, "version" for all the data sets. For example, suppose your function has *three* parameters: c, d, and e. You tag only the parameters d and e as "Shared". Suppose that you want to fit *two* data sets. In this case you will have the total of four parameters to fit: one "version" of d and one "version" of e (since d and e are shared) and two (one for each data set) "versions" of c (since c is not shared).

Starting the Fitting

To begin fitting, select **Action:Fit**. This menu command opens the Fitting Session dialog box.

The Fitting Session Concept

Note: The NLSF always reports the reduced chi^2 value, not chi^2. In some locations of the NLSF, reduced chi^2 is labeled "chi^2". In other locations, it is labeled "chi^2/DoF". In all cases the actual value is reduced chi^2.

The concept of a fitting session is important for your understanding of how Origin's nonlinear curve fitter works. At each iteration, the fitter computes the Variance-Covariance matrix using its value from the previous iteration.

This matrix depends on:

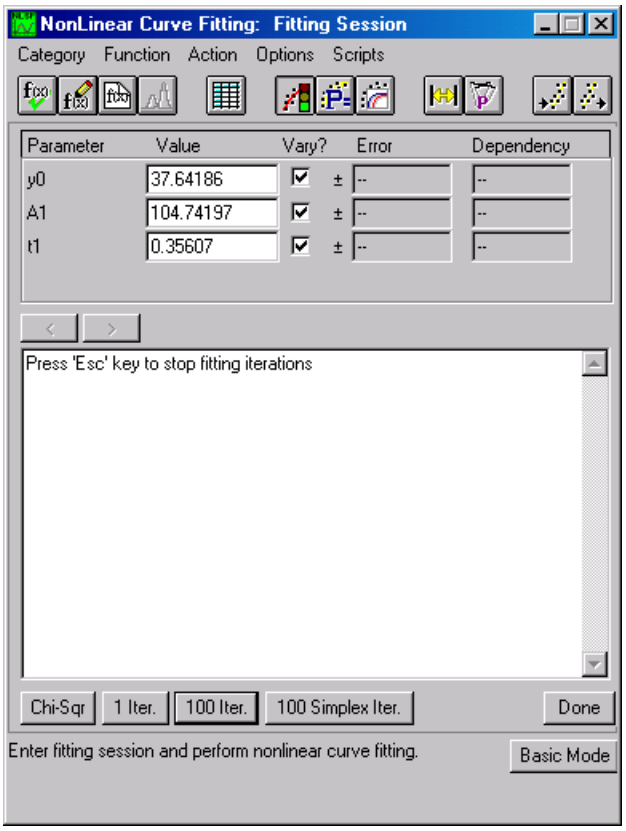
1) The fitting function.

2) The number of parameters.

3) The data set assignments.

If any of these properties are altered, the current Variance-Covariance matrix is unusable for the altered properties, which means that the fitting session has to end. When a fitting session ends, all the actions that you have selected or defined in the After Fitting dialog box are executed. Additionally, when a fitting session starts, all the actions that you have selected or defined in the Initializations dialog box are executed. To make sure that you do not inadvertently end a fitting session, Origin's nonlinear fitter prompts you for the confirmation of your action by opening an Attention dialog box.

The Fitting Session Dialog Box


NonLinear Curve Fitting: Fitting Session
Category Function Action Options Scripts
Parameter Value Vary? Error Dependency
y0 37.64186 ± -- --
A1 104.74197 ± -- --
t1 0.35607 ± -- --
Press 'Esc' key to stop fitting iterations
Chi-Sqr 1 Iter. 100 Iter. 100 Simplex Iter. Done
Enter fitting session and perform nonlinear curve fitting.
Basic Mode

The Parameter Value Text Boxes

The NLSF provides automatic parameter initialization routines for all of the built-in functions. The parameter initialization routine for the selected fitting function can be reviewed in the Parameter Initializations dialog box of the NLSF (**Scripts:Parameter Initialization**). These routines use the selected dependent and independent data sets to determine appropriate initial parameter values for the selected fitting function.

The parameter initialization routine for a selected function is automatically run when you activate the Fitting Session dialog box. When activated, the Value text boxes display initial values and the graph displays a first guess fit curve in addition to your data. You can also manually run the parameter initialization routine by 1) activating the NLSF Parameter Initializations dialog box, 2) clicking the Check button to compile the initialization routine, and 3) clicking the Execute button to run the initialization routine. After clicking the Execute button, the Init. Value text boxes should display initial parameter values.

If you are fitting multiple data sets and you have some parameters which are not shared, the different versions of these parameters are denoted with *a_#*, where *a* is the parameter.

You can edit the parameter values in the associated text boxes as desired. Every new iteration (or set of iterations) starts from these values.

The Vary Check Boxes

Each parameter contains a Vary check box. Select this check box to vary the parameter value during the iterative procedure. Otherwise, the parameter remains fixed at its current value.

The Error List Boxes

If at least one iteration has been done, these list boxes contain the estimates of the standard errors. The error is $\sigma_i = \sqrt{C_{ii}\chi^2}$, where C_{ii} is the diagonal element of the variance-covariance matrix.

The variance-covariance matrix is defined as $\mathbf{C} = \left(\mathbf{F}'\otimes\mathbf{F}\right)^{-1}$, where $\mathbf{F}$ is the Jacobian $F_{i,j} = \partial f\left(x_{1i}, x_{2i}, ...; p_1, p_2, ...\right) / \partial p_j$ (here f is the fitting function for the data set values of the independent variables $x_1 = x_{1i}$, $x_2 = x_{2i}$, ...).

The Dependency List Boxes

These list boxes display the parameter dependency. If the equation is overparameterized, there will be mutual dependency between parameters. The dependency for the *i*th parameter is defined as $1 - \frac{1}{C_{ii}C_{ii}^{-1}}$. If this value is close to one, there is strong dependency.

The Chi-Sqr Button

Click Chi-Sqr to display the reduced chi^2 value for the current parameter values. The reduced chi^2 value is displayed in the view box at the bottom of the dialog box.

The 1 Iteration Button

Click 1 Iter to perform one Levenberg-Marquardt (LM) iteration. The new parameter values are displayed in the Parameter Value text box, together with the error and dependency values.

The n *Iterations Button*

Click *n* Iter to cause the fitter to perform, at most, *n* LM iterations. Set the *n* value from the Max. Number of Iterations drop-down list in the Control Parameters dialog box.

If the tolerance is reached or an error occurs before *n* iterations have been performed, less than *n* iterations will be performed. Sometimes the actual number of iterations performed may be zero. This happens if the parameter values cannot be improved any more. The number of iterations actually performed (which improved the fit by decreasing the reduced chi^2 value) is displayed in the view box at the bottom of the dialog box.

Stop the iterations at any time by pressing the ESC key.

The n *Simplex Iter. Button*

Click this button to perform *n* Simplex iterations. Normally, you will not need to do this because the Simplex method is much less robust and reliable than the LM method. However, if the LM method for a set of data behaves poorly, try the Simplex method.

The < and > Buttons

These buttons enable you to retrieve the values of parameters which the fitter has already gone through. For example, click the < button to display the parameter values that were current before the last iterations.

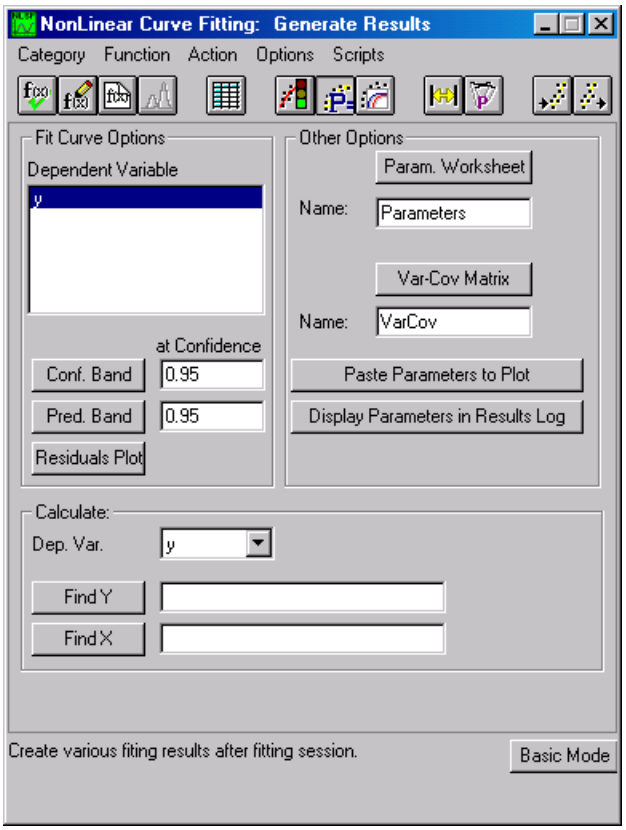
The View Box

This view box displays various quantities which change during a fitting session, including: the reduced chi^2 value, the parameter values, the error estimates, and the actual number of iterations performed (before the current iteration).

The Fitting Results

Select **Action:Results** to open the Generate Results dialog box. Edit this dialog box to create additional curves describing the results of your fitting, as well as to control the display of the fitting results. This dialog box is usually edited *after* you have found the best parameter values using the Fitting Session dialog box.

The Generate Results Dialog Box



The Create Fit Curves Group

This group enables you to create three supplemental curves for each dependent variable.

1) Confidence Band Curves

Select a dependent variable from the Dependent Var. list box. Specify the desired confidence level in the At Confidence text box. Generate the confidence band curves for the selected dependent variable by clicking the Conf. Band button.

The confidence interval for the fitting function says how good your estimate of the value of the fitting function is at particular values of the independent variables $x_1 = x_{1i}$, $x_2 = x_{2i}$, ... You can claim with $100a\%$ confidence that the correct value for the fitting function lies within the confidence interval, where a is the desired level of confidence. This defined confidence interval for the fitting function f is computed as:

$$f\left(x_{1i}, x_{2i}, \ldots; p_{1i}, p_{2i}, \ldots\right) \pm t_d^{\alpha/2}\left[\chi^2 \mathbf{f'Cf}\right]^{1/2}$$

where $\mathbf{f} = \left[\partial f / \partial p_1, \partial f / \partial p_2, \ldots, \partial f / \partial p_p\right]$, $d = n^{eff} - p$ is the number of degrees of freedom, $t_d^{\alpha/2}$ is the bi-tail t -distribution value, $\alpha = 1 - a$, and $\mathbf{C}$ is the variance-covariance matrix.

2) Prediction Band Curves

Select a dependent variable from the Dependent Var. list box. Specify the desired confidence level in the At Confidence text box. Generate the prediction band curves for the selected dependent variable by clicking the Pred. Band button.

The prediction interval for the desired confidence level *a* is the interval within which 100*a%* of all the experimental points in a series of repeated measurements are expected to fall at particular values of the independent variables $x_1 = x_{1i}$, $x_2 = x_{2i}$, ... This defined prediction interval for the fitting function f is computed as:

$$f\left(x_{1i}, x_{2i}, \ldots; p_{1i}, p_{2i}, \ldots\right) \pm t_d^{\alpha/2}\left[\chi^2\left(1 + \mathbf{f}'\mathbf{C}\mathbf{f}\right)\right]^{1/2}$$

where $\mathbf{f} = \left[\partial f / \partial p_1, \partial f / \partial p_2, \ldots, \partial f / \partial p_p\right]$, $d = n^{eff} - p$ is the number of degrees of freedom, $t_d^{\alpha/2}$ is the bi-tail t -distribution value, $\alpha = 1 - a$, and $\mathbf{C}$ is the variance-covariance matrix.

3) The Residue Plot Button

Click this button to generate the residue plot for the selected dependent variable. Residue points represent the difference between the theoretical function and the actual data points.

The Param. Worksheet Button

Click this button to create a separate worksheet containing all the results of your fitting session (parameter values, reduced chi^2 value, errors, etc.). Type the desired worksheet name in the associated text box.

The Parameters worksheet lists the following quantities:

The first n rows of the worksheet list information on the n parameters that were involved in the fitting process. For each parameter, the quantities listed in successive columns are:

a. Name: parameter name.

b. Value: Parameter value obtained in the fitting process.

c. Err: Error on the parameter value.

d. Vary: Whether the parameter was allowed to vary (floating) or was fixed by the user (fixed).

e. LLimit: Lower confidence limit on the parameter.

f. ULimit: Upper confidence limit on the parameter.

LLimit and ULimit are calculated by searching for the values of each parameter p that give an SSR(p) (minimized over the remaining parameters) greater than SSR by a factor (1+F/(N-P)).

SSR(p) = SSR * (1+F/(N-P))

Where F = Ftable(Confidence, 1, N-P) and SSR is the minimum SSR found during the fitting session.

g. Depend: Dependency of the parameter (a value very close to 1 indicates strong dependency, and therefore, over parameterization).

h. ConfIntv: Confidence interval. Calculated based on a linear approximation and is given by Standard Error * t, where t is the critical value of the t distribution for the given confidence level.

The n rows of parameter information are followed by:

a. ChiSquare: reduced chi^2 value of fit.

b. SSR: sum of squares of difference between data and fit values.

c. Correlation: correlation coefficient (R).

d. COD(R^2): Coefficient of Determination (R^2).

e. MuFinal: final value of diagonal magnification of the curvature matrix.

f. MuMin: smallest value of Mu that was ever reaching during fitting.

g. DerivStep: parameter change amount for calculating derivatives (Derivative Delta).

h. ParaChange: the number of parameters that were allowed to vary during fitting.

i. Tolerance: tolerance value to stop iterations.

j. Confidence: value for deciding confidence bands.

k. Iterations: the number of iterations performed in the last fitting operation.

l. Range1: beginning index of data range used in fitting.

m. Range2: ending index of data range used in fitting.

n. Step: incremental step size used when only a subset of data points were used in the fitting process (Ex. Step =4 means every fourth data point was used).

o. DataPoints: number of data points considered in the fitting process.

p. DOF: no. of degrees of freedom = No. of data points considered - no. of floating parameters (parameters that were not fixed).

q. Constr: the number of constraints that the user enters in the General Linear Constraints text box in the Parameter Constraints dialog box. The Enabled check box has to be selected for the constraints to be counted.

r. ConstrEff: the number of effective constraints. If you type in constraints on a parameter and then fix the parameter value (clear the Vary? check box in the Fitting Session dialog box), those constraints will not be counted.

The Var-Cov Matrix Button

Click this button to create a separate window containing the variance-covariance matrix. Type the desired window name in the associated text box.

The Paste Parameters to Plot Button

Click this button to create a label on your graph, and paste the fitting results into the label.

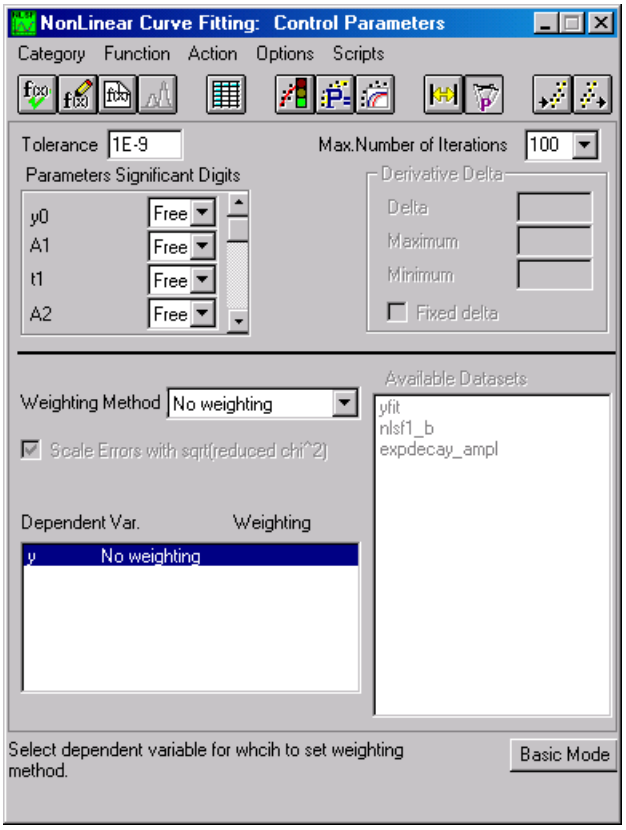
The Display Parameters in Results Log Button

Click this button to copy the results to the Results Log.

Controlling the Fitting Procedure

Select **Options:Control** to open the Control Parameters dialog box. Edit this dialog box to specify several quantitative properties of the fitting procedure. These properties directly affect the way the fitter performs iterations.

The Control Parameters Dialog Box



The Tolerance Text Box

Type a value for the tolerance in this text box.

When you click *n* Iter in the Fit Session dialog box, this causes the fitter to try to perform, at most, *n* LM iterations of reduced chi^2. If the relative change of the value of reduced chi^2 between two successive iterations is less than the value in the Tolerance text box, less than *n* iterations are performed. If you want the fitter to perform still more iterations, click on either the *n* Iter or the 1 Iter button in the Fitting Session dialog box. The *n* value is specified in the Max. Number of Iterations text box (see below).

The Max. Number of Iterations Drop-down List

Specify the value for the maximum number of iterations performed when the *n* Iter button is clicked on in the Fitting Session dialog box.

The Derivative Delta Group

This group determines how the fitter will compute the partial derivatives with respect to parameters for *user-defined functions* during the iterative procedure. The Derivative Delta group is unavailable for built-in functions as Origin's curve fitter uses analytical expressions. (Note: You can define a user-defined function with partial derivatives.)

For the user-defined functions, the derivative with respect to the parameter, p_1, is computed as (for simplicity, written for a function which has one independent variable):

$$derivative = [f(x\ ; p_1 + Delta, p_2, ...) - f(x\ ; p_1, p_2, ...)] / Delta$$

where Delta is the increment. If the Fixed Delta check box is selected, the value of Delta used in the computations is the value entered in Delta text box and is the same for all the parameters. The Maximum and Minimum text boxes are then disabled. If the Fixed Delta check box is cleared (unchecked), then the actual value of Delta for a particular parameter is equal to the current value of the parameter times the value specified in the Delta text box. In this case, use the Maximum and Minimum text boxes to specify the limiting values of the actual Delta in case a parameter value becomes too large or too small. It is recommended, at least when you start fitting your new function, *not* to select the Fixed Delta check box.

The Parameters Significant Digits Group

Select values for the display of significant digits for each parameter from the associated drop-down list. Select Free from the drop-down list to use the current Origin setting.

The Weighting Method Drop-Down List

The bottom part of the Control Parameters dialog box enables you to select how different data set points are to be weighted when computing reduced chi^2 during the iterative procedure. Select the desired weighting method from the Weighting Method drop-down list. The choices are: No weighting, Instrumental, Statistical, Arbitrary data set, and Direct Weighting. If you select the Arbitrary data set method, specify the data set which contains the weighting values for each dependent variable from the Available Datasets list box.

The Scale Errors with Sqrt(reduced chi^2) Check Box

This check box only affects the error on the parameters reported from the fitting process, and does not affect the fitting process or the data in any way.

Leave the check box selected when there are no associated error bars with the data (which is the default - and only - option). In this case, the error on the fit parameters is calculated as SQRT(cov_{ii}).

Leave the check box cleared when the data has associated error bars and a weighting method has been chosen by you. This is the default, and recommended setting for this check box. In this case, the error on the fit parameters is calculated as SQRT(cov_{ii}).

When the data has associated error bars and a weighting method has been chosen by you, you have the option to select the check box, thereby multiplying the reported error on the fit parameters by the square root of the reduced chi-squared. In this case, the error on the fit parameters is calculated as SQRT(cov_{ii}*(Chi^2/DOF)).The Dependent Var. List Box

If you selected the Arbitrary data set method from the Weighting Method drop-down list, highlight a dependent variable in this list box. Click on the desired data set name in the Available Datasets list box.

The Available Datasets List Box

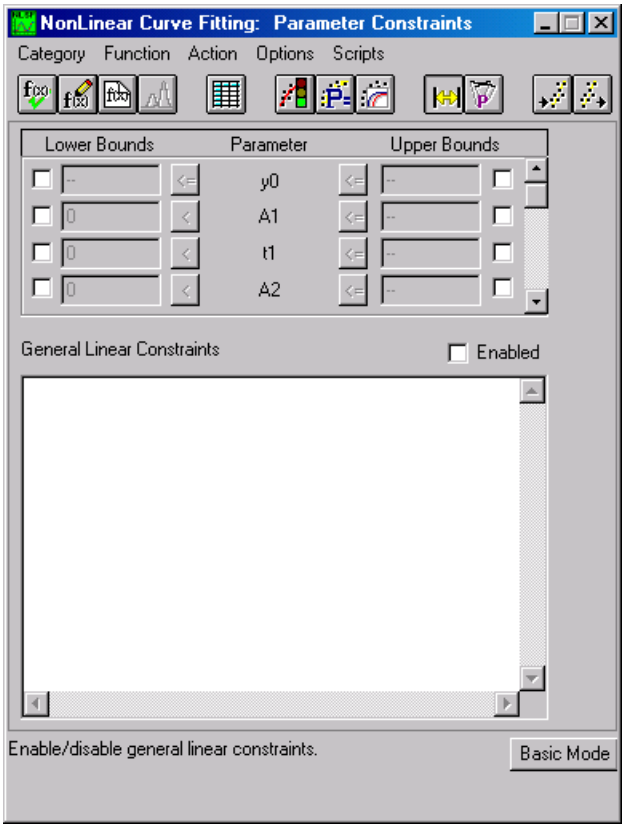
Click on the data set name in this list box after selecting the dependent variable in the Dependent Var. list box (for Arbitrary data set weighting method only).

Setting the Parameter Constraints

Select **Options:Constraints** to open the Parameter Constraints dialog box. Impose linear constraints on the parameter values in this dialog box. If the constraints are selected, the fitter chooses only those combinations of parameter values which satisfy the constraints during the iterative procedure.

Use the constraints if the fitting procedure is unstable causing the parameters to wander into wrong parameter regions. For example, in the exponential growth model $y = A\exp\left[\left(x - x_0\right)/t\right]$ the values of the parameter t close to zero may cause instabilities. A constraint such as $t \geq 0.1$ may remedy the problem.

The Parameter Constraints Dialog Box



The Lower and Upper Bounds Group

Simple constraints such as lower and upper bounds on the parameters are set in this group. The parameter names are listed in the middle of each row. The Lower Bounds and Upper Bounds text boxes contain the lower and the upper bounds. If you have not set a particular bound, the corresponding text box is empty. Edit the bounds by selecting the associated check boxes. Click the <= buttons to toggle between <= (less than or equal to) and < (less than). Type the desired value in the text box. Disable a bound by clearing (unchecking) the associated check box.

The General Linear Constraints Edit Box

Impose general linear constraints in the associated text box using the following format (assuming **a**, **b**, **c**, and **d** are parameters):

```
a>b;
a+2*b>=c*2-d;
```

```
a<b<c;
a/3<9
```

If there is more than one constraint, separate constraints by a semicolon.

To change lines, press CTRL+ENTER.

The following constraints are invalid as they are nonlinear:

```
a^2>c;
a*b>3;
1/b>c+2;
sin(a)<c
```

Five relational operators are supported: =, <, <=, >, and >=. The curve fitter treats < and <= the same. Likewise > and => are treated the same (this is not true for simple constraints, see above).

You can place multiple operators in a single sentence, such as:

```
4<a<b<6
```

which is equivalent to:

```
4<a; a<b; b<6
```

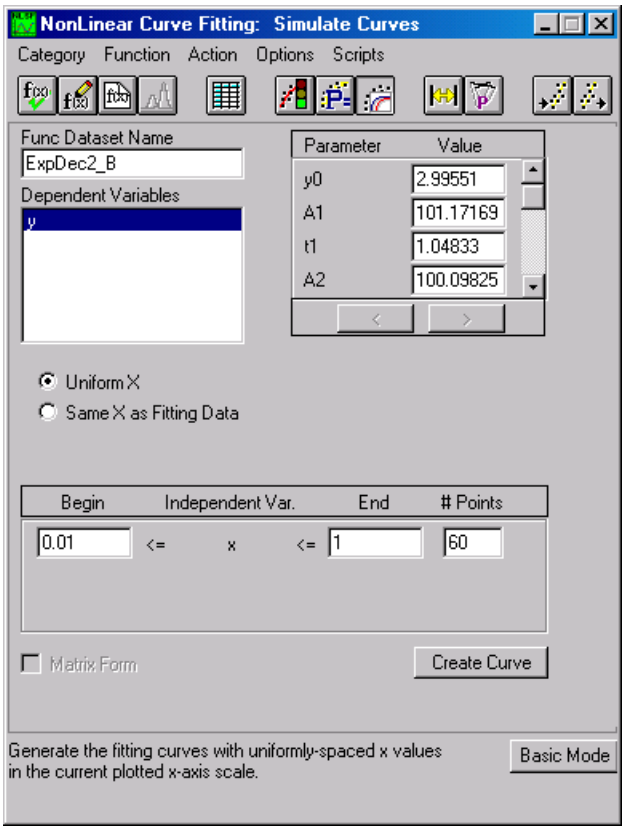
Coefficients need not be numeric constants. However, they must evaluate to valid numbers. For example, if the function has two parameters, P1 and P2, you can use a linear constraint such as P1+qw*P2 assuming that you have previously given qw a numeric value.

Temporarily disable constraints by clearing (unchecking) the Enabled check box. Constraints take effect only if the Enabled check box is selected.

Simulation of Data

Select **Action:Simulate** to open the Simulate Curves dialog box. Features provided in this dialog box are useful when you are uncertain about the initial values of parameters for fitting. You can plot the theoretical function for any parameter values in order to compare the curve with the data. This enables you to get an understanding of which parameter values produce curves that "look like the data". This is important because reasonably good starting parameter values are in most cases a precondition for the success of the fitting.

The Simulate Curves Dialog Box



The Func Dataset Name Text Box

This text box displays the name of the data set which will contain the theoretical data points to be generated.

The Dependent Variables List Box

All the dependent variables are displayed in this list box. Click to select a variable to be plotted.

The Parameter Group

The names of all the parameters are displayed in the list box. Set the parameter values used for plotting the theoretical curve in the associated text box. Click the < and > buttons to browse through the sets of parameter values for which you have already created curves. If you select **Action:Fit**, the last set of parameter values selected in this dialog box are carried over to the Fit Session dialog box, which enables you to start fitting from these values.

The Begin/End Group

Determine how to plot the theoretical curves for the simulation in the Begin/End group. All independent variables are listed in this view box. Set the lower and the upper limit of the independent variable values by editing the associated Begin and the End text boxes. Select the number of theoretical points in the associated # Points text box. If there is more than one independent variable, than the # Points text boxes for different independent variables must contain the same number. Origin's fitter generates theoretical curves as follows:

1) One data set (or column in a worksheet) is created for each independent variable. The number of rows is the same for all of the data sets (columns).

2) The fitter takes the independent variable values from a row, computes the values of the dependent variable(s), and displays them. The process is repeated for each row.

The Create Curve Button

Click Create Curve to generate the curve.

The Matrix Form Check Box

This check box applies only if there is more than one independent variable. If the check box is selected, the theoretical curve will be simulated on a grid. Note that this way of simulating curves requires much more computer memory (for example, if you have specified 60 points for each of the *three* independent variables, the use of Matrix Form will create 60x60x60 values, rather than only 60).

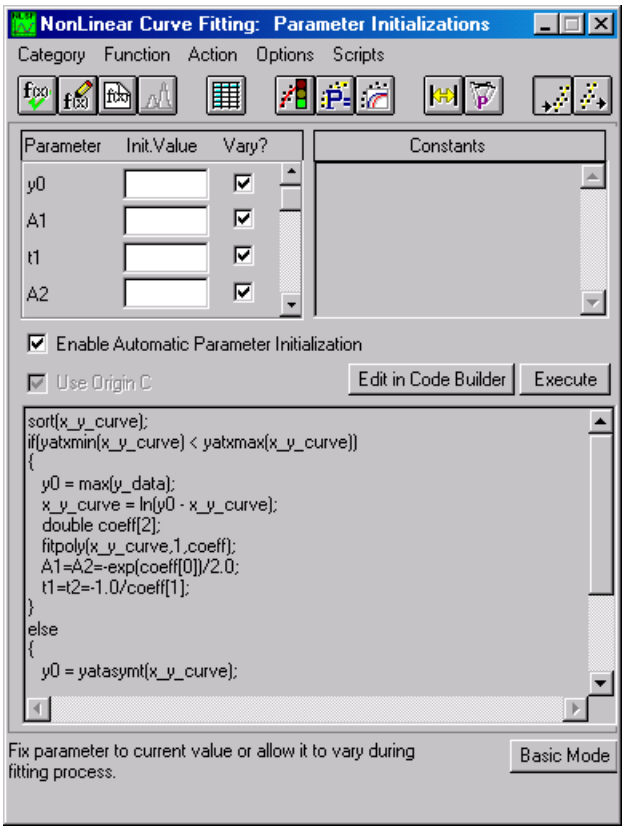
Running Scripts at Specified Triggers

Parameter Initialization

Select **Scripts:Parameter Initialization** to open the Parameter Initializations dialog box.

Note: If the version you are upgrading includes a user-defined fitting function with LabTalk script defined in the pre-7 Initializations dialog box of the NLSF, then this script will be accessible from the Before Fitting dialog box (**Scripts:Before Fit**) in the version 7 NLSF. Any Origin C code or LabTalk script that you enter on the Parameter Initializations dialog box will be executed after the Before Fitting script when you activate the Fitting Session dialog box.

The Parameter Initializations Dialog Box



The Parameter Group

The NLSF provides automatic parameter initialization routines for all of the built-in functions. The parameter initialization routine for the selected fitting function can be reviewed in this dialog box. These routines use the selected dependent and independent data sets to determine appropriate initial parameter values for the selected fitting function.

The parameter initialization routine for a selected function is automatically run when you activate the Fitting Session dialog box. When activated, the Value text boxes in the Fitting Session dialog box display initial values and the graph displays a first guess fit curve in addition to your data.

You can also manually run the parameter initialization routine from this dialog box by 1) clicking the Check button to compile the initialization routine, and 2) clicking the Execute button to run the initialization routine. After clicking the Execute button, the Init. Value text boxes should display initial parameter values.

You can also edit these parameter values as needed.

The Constants Text Box

If your function contains constants other than the parameter names and the independent or dependent variables, and the values of those constants are not specified in the function definition script or outside the fitter (for example, in the Script window), define these constants in the Constants text box. When you define the constants in this field, you will never have to set them as fixed, because they are automatically set.

The proper procedure to follow when using the Constants text box is to first define your function with the constant parameter names in it using the fitter's Define New Function dialog box. When you type your parameter names in the Define New Function dialog box, do not include the constant parameter names. Instead, define the constant parameters in the Constants text box (in the Initializations dialog box). Enter the constant parameters in this field as follows: c0=2; <Enter> c1=3; <Enter> and so on. In other words, each constant term and its associated value should be separated by a semicolon (;). When the fitting process is performed the constants terms will automatically be figured into the calculation, but will not show up in the parameter list for initialization since they are already initialized and set as fixed by entering them into the Constants Field.

Note: The following numeric system variables should not be used as constant names: X1...Xn, Y1...Yn, Z1...Zn, and the letter i. There are also LabTalk system variables which should be avoided. For more information on these system variables, see the LabTalk Help file. Furthermore, the letters T, J, and E should be avoided. As a result of these limitations, it is suggested that constant names contain more than one character.

The Initialization Scripts Text Box

For user-defined fitting functions, you can write your own initialization routines in this text box. If you enter Origin C code (versus LabTalk), you must select the Compile check box so that the routine gets compiled when you activate the Fitting Session tab. You can also click the Check button to immediately compile the routine to check for syntax errors. The Execute button runs the parameter initialization routine and initializes the fit parameters. Additionally, the routine is automatically run when you activate the Fitting Session tab.

For help in writing the Origin C parameter initialization routine for your user-defined function, review the initialization routines provided with the built-in functions. You can review them in the NLSF or you can review the [Parameters Initialization] section of the built-in function's .FDF file. The parameter initialization routines for the built-in functions call Origin C functions that are defined in the internal.c source file which is located in your Origin \ORIGINC\SYSTEM subfolder. To review these functions, open internal.c in Code Builder (click the Code Builder button on Origin's Standard toolbar and then click the Open button). Notice that some functions such as `sort`, `smooth`, and `xatymin` take a `Curve` as an argument. Other functions such as `min` take a `Dataset` as an argument.

To pass a `Curve` to a function, use the notation *`independentVar_dependentVar`*`_curve`. For example, if your independent variable is named position and your dependent variable is named amplitude, then pass a `Curve` to the function using the argument `position_amplitude_curve`.

To pass a `Dataset` to a function, use the notation *`independentVar`*`_data or` *`dependentVar`*`_data`. For example, if your dependent variable is named amplitude, then pass a `Dataset` (in this case, the dependent variable) to the function using the argument `amplitude_data`.

For more information, see the Programming Guide Help file.

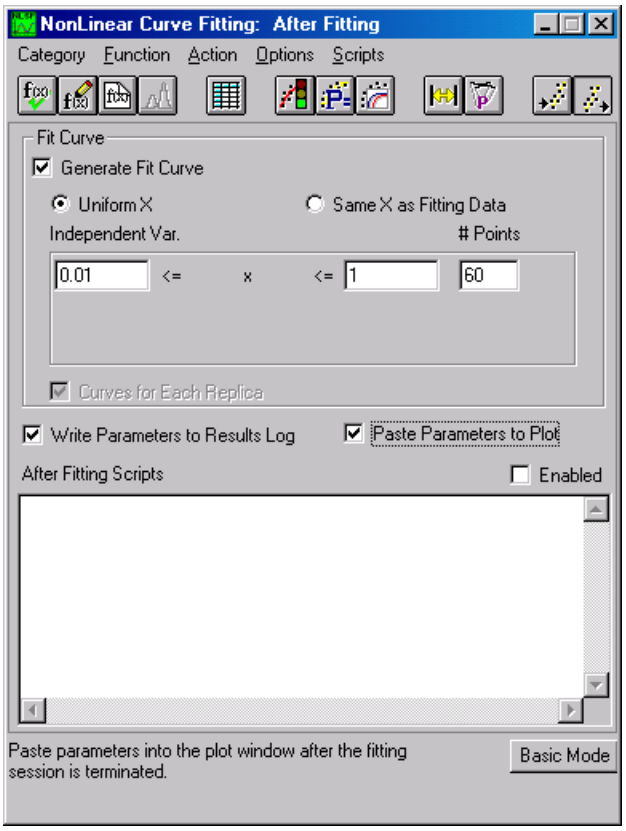
Note: For built-in and user-defined fitting functions that include parameter initialization routines: If a fit drifts off during the minimization process, re-select the Parameter Initializations tab and click the Execute button. This action re-runs the parameter initialization routines and resets the fit.

After Fitting

Select **Scripts:After Fit** to open the After Fitting dialog box. Edit this dialog box to define what you want Origin's nonlinear curve fitter to do when *ending* a fitting session.

Note: You cannot enter Origin C routines in this dialog box - only LabTalk is allowed. However, you can compile an Origin C function in Code Builder and then call that function using LabTalk. For more information on Origin C, see the Programming Guide Help file.

The After Fitting Dialog Box



The Fit Curve Group

Select the Generate Fit Curve check box to create a new data set which contains the theoretical curve points and display the curve on the graph. Select the X data set source from the associated radio buttons.

Uniform X means that the fitter chooses equidistant points.

Same as X Fitting Data means that the curve is created for the points contained in the original data.

Select the Curves for Each Replica check box to create a separate curve for each replica. The number of replicas is set in the Replicas dialog box.

Note: If you clear the Generate Fit Curve check box and later end the fitting session, the fitting curve that is displayed during the iterative process will be erased.

The Write Parameters to Results Log Check Box

Select this check box to send the fitting results to the Results Log when ending a fitting session.

The Paste Parameters to Plot Check Box

Select this check box to create a label on your graph and paste the fitting results onto it when ending a fitting session.

The After Fitting Scripts Text Box

Type a LabTalk script in this text box for execution when ending a fitting session. For example, if you want the fitting results displayed or stored in a particular manner, write a script which performs the task and enter it in this text box.

The script entered in the Scripts After Fitting text box is executed when ending a fitting session only if the Enabled check box is selected.

Before Fitting

Select **Scripts:Before Fit** to open the Before Fitting dialog box. Edit this dialog box to define what you want Origin's nonlinear curve fitter to do when *starting* a fitting session.

Note: You cannot enter Origin C routines in this dialog box - only LabTalk is allowed. However, you can compile an Origin C function in Code Builder and then call that function using LabTalk. For more information on Origin C, see the Programming Guide Help file.

Type a LabTalk script in the Scripts to Execute Before Fitting text box for execution when entering a fitting session. The script in this text box will execute before any scripts in the Initializations dialog box. However, you must select the Enabled check box for the script to execute.

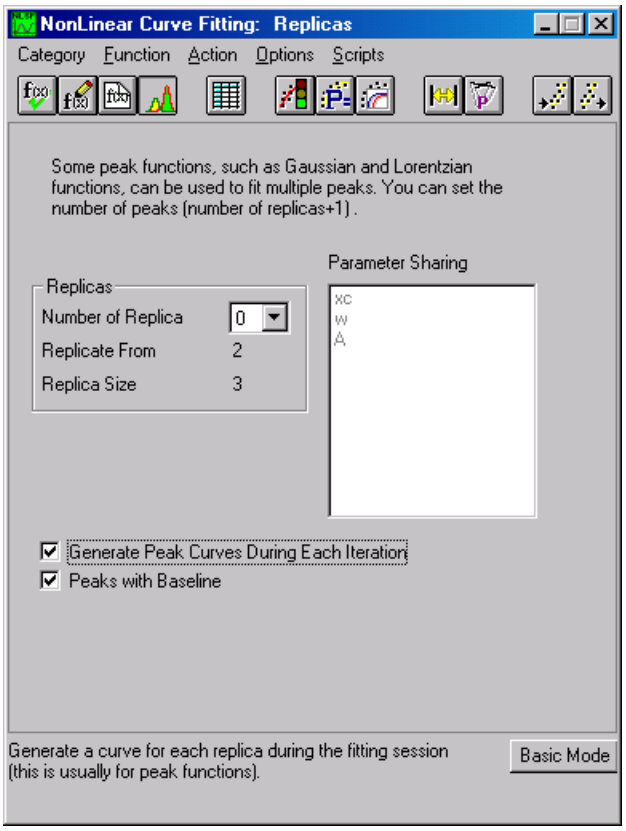
Upgrade Note: If the version you are upgrading includes a user-defined fitting function with LabTalk script defined in the pre-7 Initializations dialog box of the NLSF, then this script will be accessible from this dialog box (**Scripts:Before Fit**) in the version 7 NLSF.

Fitting Multiple Peaks with Replicas of the Function

Select **Options:Replicas** to open the Replicas dialog box. Edit this dialog box to fit your data to some of the built-in peak functions by replicating the function into several "copies", each of which may have different parameters. Use this feature if you believe that your data contain multiple peaks of the same sort (say, Lorentzian) but different centers and/or widths. If the function you have selected does not support replications, this dialog box is disabled.

Edit this dialog box to fit your data to some of the built-in peak functions by replicating the function into several "copies", each of which may have different parameters.

The Replicas Dialog Box


NonLinear Curve Fitting: Replicas
Category Function Action Options Scripts
Some peak functions, such as Gaussian and Lorentzian functions, can be used to fit multiple peaks. You can set the number of peaks (number of replicas+1).
Parameter Sharing
Replicas
Number of Replica
0
Replicate From
2
Replica Size
3
xc
w
A
Generate Peak Curves During Each Iteration
Peaks with Baseline
Generate a curve for each replica during the fitting session (this is usually for peak functions).
Basic Mode

The Replicas Group

Select the number of replicas ("copies") of the function that you want to use in fitting from the Number of Replicas drop-down list. You must set the number to n - 1, where n is the number of peaks you believe are present in your data.

The Replicate From value shows which parameters are used for fitting multiple peaks for the particular function. For example, in the case of a Gaussian function the parameters are ordered as: *y0, xc, w,* and *A* in the function definition file. If the value of Replicate From is two, that means that the parameters, beginning with the second one (*xc*), will be used in replicas, whereas there will be only one value of the first parameter (*y0*).

The Replica Size is the number of parameters used in replicas.

The Parameter Sharing List Box

Specify if you want some of the parameters in the replicate unit to have the same value for all the peaks by tagging those parameters as shared. Tag a parameter as shared by double-clicking on its name in the

Parameter Sharing list box. The meaning of parameter sharing (here) is the analogous to the same feature when fitting multiple data sets.

The Generate Peak Curves During Each Iteration Check Box

Select this check box to display the peak curves for each replica after every iteration.

The Peaks with Baseline

Select this check box if you want each peak curve to be plotted from the common vertical offset.

Initializing the Fitter

Select **Action:Initialize** to initialize the fitter. This action should be performed after you are done fitting the current data set and before starting a new fitting process in another data set. The initialization resets all settings under the various menu options to the default values. You need not perform this operation if you are fitting subsequent data sets with the same fitting function, and would like to retain your settings under various menu options.

Using the Fitter with the Network Version of Origin

An Origin client can modify or create a fitting function. If the created function has the same name as a server fitting function, the client function is used for fitting.

To define a new fitting function on an Origin server so that clients can use it, perform the following:

1) Run the server and create the new fitting function.

2) On the server, rename the created *.FDF file (in the \FITFUNC folder) from *User#*.FDF to *NewName*.FDF where *NewName* is descriptive of the function.

3) In the server's NLSF.INI file, change the default FDF file name for the newly created fitting function from *User#* to *NewName*, where *NewName* is the same descriptive file name.

4) Copy this line you just modified:

New Function Name = NewName

from the server's NLSF.INI file to the client's NLSF.INI file, under the same [FunctionGroup] section.

The client can now use this server-defined fitting function.

Fitting Strategies

Do I need NLSF?

Before even starting Origin's nonlinear least squares fitter (NLSF), you must determine if you actually need it. If you want to fit a function, such as:

$$y = p_1 \sin(x) + p_2 x$$

you may be tempted to use NLSF since the function is obviously nonlinear. However, Origin's NLSF is primarily intended for use with functions which depend *nonlinearly* on at least one of its *parameters*. Since the above function is linear in the parameters, you may be better off trying (multiple) linear regression, which is also supplied with Origin.

Using the Built-in Functions

Before deciding to define your own function, make sure that the function you need is not already among the built-in functions. This is very important because of the way the Levenberg-Marquardt chi^2 minimization is implemented in Origin's NLSF. For user-defined functions, in each iterative step the NLSF computes partial derivatives of the fitting function(s) with respect to parameters in all the data set points. For built-in functions, Origin's NLSF uses built-in analytical derivatives for the computation of the derivatives, which is more reliable than straightforward numerical computation of the same derivatives. (Note: You can define a user-defined function with partial derivatives.)

Parameter Initialization

An indispensable part of any fitting procedure is a good choice of initial parameter values. The NLSF provides automatic parameter initialization routines for all of the built-in functions. The parameter initialization routine for the selected fitting function can be reviewed in the Parameter Initializations dialog box of the NLSF (**Scripts:Parameter Initialization**). These routines use the selected dependent and independent data sets to determine appropriate initial parameter values for the selected fitting function.

The parameter initialization routine for a selected function is automatically run when you activate the Fitting Session dialog box of the NLSF (**Action:Fit**). When this dialog box is activated, the Value text boxes display initial values and the graph displays a first guess fit curve in addition to your data. You can also manually run the parameter initialization routine by 1) activating the NLSF Parameter Initializations dialog box, 2) clicking the Check button to compile the initialization routine, and 3) clicking the Execute button to run the initialization routine. After clicking the Execute button, the Init. Value text boxes should display initial parameter values.

You can also check and improve initial parameter values using the Simulate Curves dialog box of the NLSF (**Action:Simulate**). Use this dialog box to plot your theoretical function for any choice of parameters. Thus, you can easily compare your data with the theoretical function for any choice of parameter values. When you find a set of parameter values that generates the curve which closely resembles the data, start the iterative procedure from those values.

When the Fitting Procedure Does Not Converge

Nonlinear least squares fitting is essentially the minimization of a function of several variables (in this case, the variables the reduced chi^2 function depends on are the parameters of the fitting function). The aim of the minimization procedure is to find the *absolute* minimum of reduced chi^2. There are several reasons for the minimization procedure to have problems reaching the absolute minimum.

Relative Minimum Reached

It is not uncommon for the iterative procedure to find a relative, rather than absolute, minimum. In this case, the procedure actually converges in the sense that further decrease of reduced chi^2 seems impossible. The biggest problem is that you do not even know if the routine has reached an absolute or a relative minimum. The only way that you can "make" the iterative procedure get to an absolute minimum is to try to start fitting from several different initial parameter values and see what happens. If you always get the same final result, the result is less likely to represent a local minimum.

Parameter Values Keep Changing

The most common problem that arises in nonlinear fitting is that no matter how you choose the initial parameter values, the iterations cannot seem to converge in the sense that some, or all, parameter values keep changing with each iteration and eventually diverge producing arithmetic overflow or underflow. This should be a signal for you to do something about the fitting function and/or data you are using. There is simply no one set of parameter values which fits the data best, but rather a continuum of the values.

Overparameterized Function

Here is a typical example:

y=A*exp(x-x0);

No matter what kind of data you have, the iterative procedure will never be able to find a minimum because you have too many parameters! Rewrite your function as:

y=B*exp(x);

where B=A*exp(-x0). In other words, if, during the fitting procedure, the values of A and x0 change so that the combination B=A*exp(-x0) remains the same, the reduced chi^2 value will not change. Any attempt to further improve the fit is a waste of time. There are two simple indications that something is wrong:

1) The parameter error, as displayed in the parameter list in the Fitting Session dialog box, is very large relative to the parameter value. For example, if the width of the Gaussian is **0.5** while the error is **10**, the result for the width is meaningless since no convergence has been reached.

2) The parameter dependence (for one or more parameters) is very close to one. This is a certain indication that you have to remove (or fix) one of the parameters whose dependency is close to one since the fit does not depend on the parameter (or a combination thereof) very much.

Bad Data

Even when the function is not theoretically overparameterized, the iterative procedure may behave as if it were, due to the fact that the data do not contain enough information for some or all of the parameters to be

determined. This usually happens when the data are available only in a limited interval of the independent variable(s). For example, if you are fitting a nonmonotonous function such as Gaussian to the data which are monotonous, the NLSF will have a difficult time determining the position of the center, or the width of the peak, since the data obviously describe only one side of the Gaussian peak.

Using Constraints

When trying to reach the reduced chi^2 minimum, the Levenberg-Marquardt method carefully chooses the path in the parameter space which should lead to the minimum. However, there are situations when good initial parameter values are hard to find and a small departure can cause the fitter to wander away from the minimum without being able to come back. To prevent that, you may impose linear constraints on the parameters. For example, if you believe that the reduced chi^2 minimum for a particular case of Gaussian fit corresponds to the Gaussian width being greater than 0.1, you can prevent the fitter from trying too small values of the width **w** by imposing a constraint **w>0.1**. Since too small values of the width can easily cause an arithmetic underflow, you may improve the stability of the iterative procedure.

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